

# CAPEC Research Report 2009

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*Publication date:*
2009

*Document Version*
Publisher's PDF, also known as Version of record

# PEC09-25
# CAPEC Research Report – 2009
## Computer Aided Product-Process Engineering Center

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**June 2009**


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## Preface

This report provides an overview of our research activities and achievements for the period June 2008 to June 2009. An overview of the active research projects is provided in terms of PhD-projects, MSc- & BSc-level exam-projects, post-doctoral and other research projects. A brief overview of the CAPEC software is also included in this report.

During the period of this report, Dr. Gurkan Sin has joined CAPEC and DTU Chemical Engineering as a permanent faculty member. Professor Sten Bay Jørgensen, a co-founder of CAPEC, will be retiring at the end of June 2009 (we thank him for his valuable contributions to the founding and further development of CAPEC). The research areas of Dr. Sin overlap with that of Prof Jørgensen. More specifically, Dr. Sin will be working on systematic methods and tools for understanding, design, operation and control of (bio)chemical processes; modeling, control & system identification; uncertainty theory (global uncertainty/sensitivity analysis) & risk assessment; probabilistic-based design paradigm; and, applications in biotechnology, pharmaceutical and water industry .

A number of PhD-projects have been finalized during the period of this report while an equal number of new projects have been started. More specifically, Jakob K Huusom, Søren P Brier, Hugo E Gonzalez-Villalba and Ricardo Rodriguez-Morales have successfully defended their PhD-theses while Alicia Roman-Martinez, Chutima Swangkotchakorn, Noor A F Abdul Samad, Martina Heitzig, Philip Lutze and Azizul A B Mustafa have started new PhD-projects. A brief description of all the currently active PhD-projects can be found in this report.

Collaboration with our member companies has helped us to apply our research results to interesting industrial problems, to get valuable feedback from them and to plan future projects. Collaboration with our friends from academia has helped us to develop more comprehensive CAPE methodologies and techniques. We appreciate these collaborations and we thank our industrial and academic partners for their valuable contributions.

We would also like to acknowledge the financial support in the form of membership fees from our member companies. For funding of PhD and post-doctoral research projects we would like to thank the Danish funding agencies FTP, NABIT, EFP and ATV and the EU-research programs under FP-6 and FP-7. In addition, we would like to thank the following member companies for financial support and/or collaboration in research: Alfa Laval Copenhagen, Syngenta, AstraZeneca, Novozymes, AkzoNobel, GlaxoSmithKline, and the FMC Corporation.

Finally, we take this opportunity to thank all co-workers of CAPEC for their hard work and dedication. The CAPEC research results highlighted in this report are their achievements. This is the 11th year since CAPEC was established.

For more information about CAPEC, please contact Mrs Eva Mikkelsen (eva@kt.dtu.dk).

Rafiqul Gani 2 June 2009

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## 1. Introduction

Research in CAPEC is organized in terms of six research programs (see Fig 1.1). At the inner most level (research programs A, B), the topics are related to fundamental research while at the outer most level (E), the topics are related to applied research. In the intermediate levels (C, D), systematic model-based algorithms, methods and tools are developed by employing the results from the inner levels for use in applied research in the outer level. Since all research programs need numerical tools and databases, research program F supplies this need to all levels.

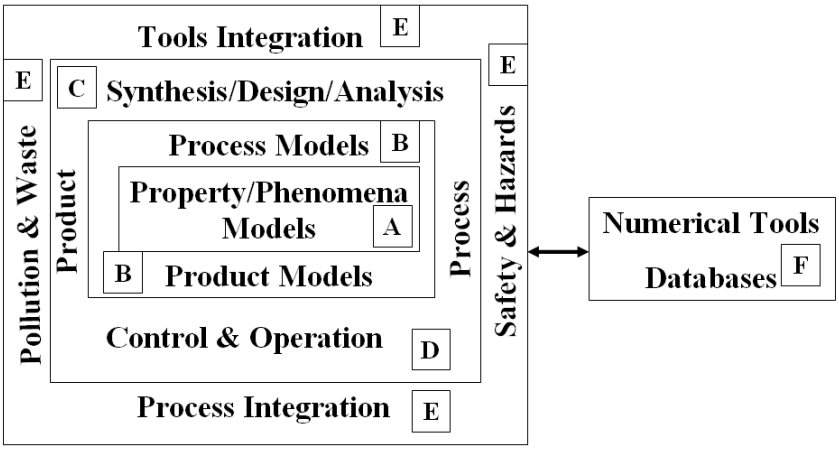



Figure 1.1: Organization of research in CAPEC in terms of research programs

The six research programs are briefly described below:

- *Research Program A – Property and Phenomena Modelling*: deals with theoretical as well as experimental studies of properties (pure component and mixture) of chemical systems and phenomena such as permeability through membranes, reaction kinetics and mass transfer through diffusion. Library of group contribution based models for a wide range of properties of organic chemicals is one of the highlights of program A.
- *Research Program B – Process-Product Modelling and Simulation*: deals with the development of models and model-based simulation systems for prediction of the behaviour and performance of a wide range of chemical and biochemical processes (operating in batch, fed-batch and continuous modes of operation) and a wide range of chemicals based products. A computer-aided modelling system for efficient model development and a collection of process-product models of various types, forms and scales are some of the highlights of program B.
- *Research Program C - Synthesis, Design & Analysis*: deals with development and use of systematic algorithms, methods and tools for synthesis, design and analysis of chemical and biochemical processes and chemicals based products. Techniques such as computer aided molecular and/or mixture design (CAMD), and, process flowsheet design (CAFD) using the reverse approach are some of the highlights of program C.
- *Research Program D - Process Control, Operation & Monitoring*: deals with the development of use of systematic algorithms, methods and tools for process control, operation and monitoring, including process analytical technologies. Techniques for tuning of controller parameters in model predictive control and methods for design of PAT systems are some of the highlights of program D.
- *Research Program E - Process and Tools Integration*: deals with on-line (process) and off-line (tools) integration as well as safety & hazards, sustainability analysis, and integration of process design-control, process-product design and process-process.

Integrated software such as ICAS, virtual process-product design lab, SustainPro and their associated methodologies are some of the highlights of program E.

- *Research Program F - Database and Numerical methods*: since CAPEC software needs to be self-sufficient in all respects for use by the industrial consortium companies, CAPEC also maintains a library of numerical methods and databases (properties of chemicals, reaction synthesis, membranes, and analysis equipments). The other research programs benefits from this in terms of data for modelling and improved simulation strategies.

Based on the above, the research objectives of CAPEC can be summarized as:

> *Develop computer-aided systems for efficient and reliable process simulation; for systematic synthesis, design and analysis of sustainable chemical products and their manufacturing processes; for robust control, operation and monitoring of processes from principally chemical, petrochemical, pharmaceutical and biochemical industries. The computer-aided systems are to be developed based on fundamental and/or data-based modelling studies that incorporate correlation and estimation of thermo-physical and phase equilibrium properties as well as modelling the underlying principles / behaviour of the process-product.*

CAPEC's strengths can be summarized in terms of its research focus (pioneering work in certain research areas), industrial collaboration (dissemination of research results), and contacts (ability to influence developments within chemical engineering and PSE).

CAPEC's research is focused (development of generic systematic methods and tools for solution of problems related to product-process engineering) while the application horizon is wide (oil and gas, petrochemical, chemical and specialty chemical, pharmaceutical, food and bio industries). More specifically, CAPEC's contribution in the area of group contribution based thermodynamic property modelling, computer-aided molecular-mixture design, targeted reverse approach for product-process design, systematic computer-aided methods and tools for modelling, design, analysis and control are well known within the PSE community.

Through CAPEC's large industrial consortium (consisting of 29 member companies – see Appendix for a list of member companies), CAPEC coworkers have the unique opportunity to get quick and useful feedback on their developed models, methods and tools as well as insights to the current and future needs of the various industrial sectors represented by the industrial consortium members.

The dissemination of the research results of CAPEC is carried out in terms of:

- *Computational Tools*. Predictive models for reliable property estimation for a wide range of chemicals; generic mathematical models for process operation, product performance; computer-aided tools for product-process synthesis & design, etc., are used by leading industries and close to 50 universities from all over the world.
- *Technology*: Developed systematic methodologies for process-product synthesis, design, analysis and control (& operation), simulation strategies, solvent selection (& design), pollution prevention, sustainable process-product alternatives, etc., are routinely used to solve industrial problems and in education.
- *Application*: Industrial case studies, tutorial case studies, technology transfer studies and consulting.

Figure 1.2 (shown below) highlights the scope and significance of CAPEC's research in terms of the industries where the developed methods and tools are applicable.

| CAPEC Research Programs | Application of Research Results in terms of Industry | | | | | |
|---|---|---|---|---|---|---|
| | Petro-chemicals[1] | Chem-icals[2] | Pharma-ceutical | Agro-chemical | Bio & Food | Aroma |
| A: Property & Phenomena Modelling | | | | | | |
| B: Product & Process Modelling | | | | | | |
| C: Synthesis, Design & Analysis | | | | | | |
| D: Control, Operation & Monitoring | | | | | | |
| E: Process & Tools Integration | | | | | | |
| F: Databases & Numerical Methods | | | | | | |

| | | | | |
|---|---|---|---|---|
| Well developed methods & tools available* | Available methods & tools can easily be adapted if not directly applicable* | Available methods & tools applicable to only a small number of problems* | Needs development* | Work done during 2007-2008 |

Figure 1.2: Scope and significance of CAPEC research results shown in terms of industries where they can be applied (1: Includes also oil & gas industries; 2: includes also specialty chemicals; * Solving problems in process modelling, simulation, design, analysis and control)

## 2. Organization of Activities

The organization of educational and research activities within CAPEC are conducted by CAPEC faculty members together with the researchers and students associated with them. Figure 2.1 highlights these activities, where it can be noted that the research results coming out of the six research programs of CAPEC are disseminated in education and industry.

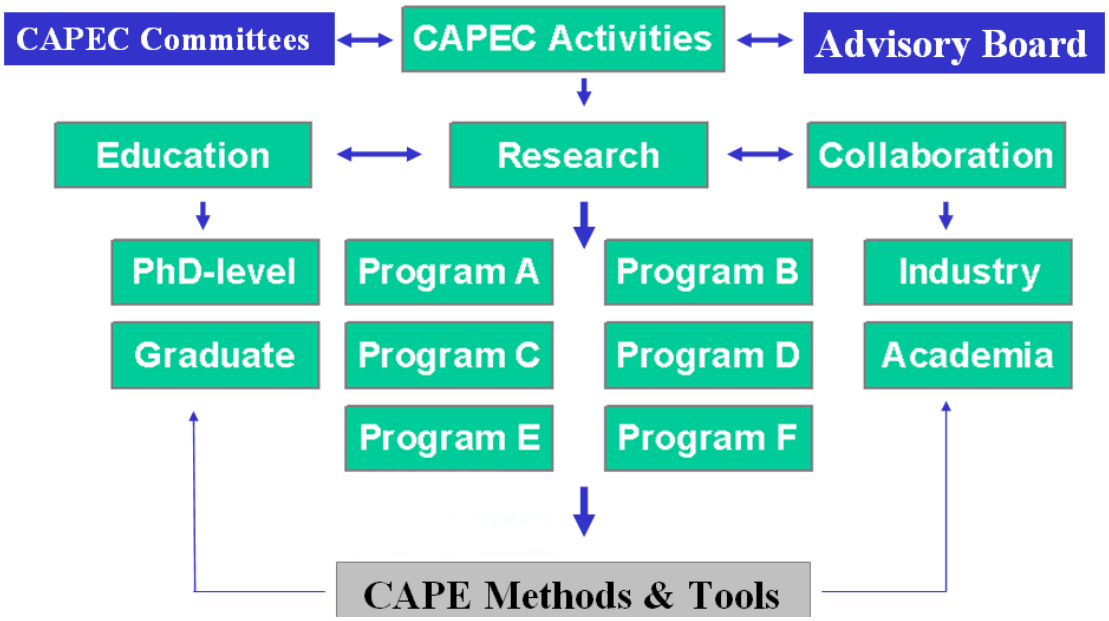



Figure 2.1: Organization of educational and research activities within CAPEC

## 2.1 CAPEC Permanent Members

**Associtae Professor Jens Abildskov (JA)**

- Research areas (A, B, C, D, F)
    - Physical/Thermodynamic Properties Modelling
    - Polymers, Solvents, Enzymes, Solids, Gases
    - Group Contribution Methods
    - Molecular Simulation
    - Product/Process Modelling

**Reader Karsten Clement (KHC)**, Director of BSc Study Program (Chemistry & Chemical Engineering)

- Reasearch areas (B, D)
    - Modelling & control

**Professor Rafiqul Gani (RaG)**, Director and Co-founder of CAPEC

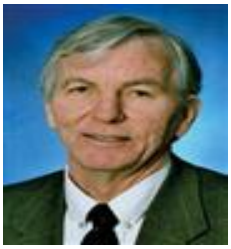
- Research areas (A, B, C, D, E, F)
    - Modelling (chemical processes and their operations, chemical products and their behaviour/properties)
    - Synthesis, design and analysis of chemical products and their processes (CAMD and CAFD)
    - Process integration (sustainable process design)
    - Tools integration and software architecture
    - Applications in petrochemical, chemical, specialty chemical, agrochemical, food and pharmaceutical industries

**Eva Mikkelsen (EVA)**

- Administrative secretary

**Associate Professor Gunnar Jonsson (GJ)**

- Associate member of CAPEC
- Research areas (A, B, C, E)
    - Membrane Technology; membrane formation and structure; membrane module design; membrane bioreactors; integration of reaction-separation
    - Transport mechanisms and selectivity; polarisation and fouling phenomena
    - Industrial Applications



**Professor Sten Bay Jørgensen (SBJ)**, Co-founder of CAPEC

- Research areas (B, C, D, E)
    - Design, Modelling & Operation of biochemical and chemical products and processes
    - Fixed and moving bed reactors; Bioreactors; Heat integrated distillation; Integrated bioreactor and membrane separation
    - Methods and tools for modelling product and process functionality aimed at Alarm system design, Hazop studies and integration of design and control

**Assistant Professor Gürkan Sin (GSI)**

- Research areas (B, C, D, E)
    - Systematic methods and tools for understanding, design, operation and control (bio)chemical processes
    - Modeling, control & system identification
    - Uncertainty theory (global uncertainty/sensitivity analysis) & risk assessment
    - Probabilistic-based design paradigm
    - Applications in biotechnology, pharmaceutical and water industry

## 3. Research Projects

### 3.1 List of current research projects

Research at CAPEC is conducted through research projects at various levels: post-doctoral, PhD, MSc, BSc and visitor-collaboration projects. Table 3.1 provides a list of the currently active projects.

Table 3.1 Currently active research projects at all levels

| **PhD-Projects (Current)** | | | | | | | |
|---|---|---|---|---|---|---|---|
| **No.** | **Area** | **Personnel** | **Project Title** | **Supervisor** | **Start** | **End** | **Funding** |
| A-50 | C, E | Jamal El. Ali Rashed | Model-based retrofit design and analysis of petrochemical processes | RaG | 1-2006 | 12-2008 | Libya |
| A-53 | A, C | Kavitha Chelakara Satyanarayana | Molecular design using grid technology | JA/RaG | 6-2006 | 5-2009 | NABIIT-DK |
| A-54 | B, D, E | Ravendra Singh | Model-based computer aided framework for design of process monitoring and analysis systems | RaG/KVG | 9-2006 | 8-2009 | DTU |
| A-55 | B, C | Merlin Alvarado Morales | Process-product synthesis, design and analysis through the group-contribution approach | RaG/JW/ KVG | 3-2007 | 2-2010 | DTU |
| A-56 | C, D, E | Mohd. Kamaruddin Bin Abd. Hamid | Integration of modelling, design and control for efficient operation of chemical processes | RaG/GSI | 6-2007 | 5-2010 | Malaysia |
| A-57 | A, B, C | Elisa Conte | Innovation in integrated chemical product-process design: Development through a model-based systems approach | RaG/JA | 7-2007 | 6-2010 | DTU |
| A-58 | B, C | Oscar Andres Prado Rubio | Modelling and optimization of integrated bioreactor and membrane separation processes | GJ/SBJ | 6-2007 | 5-2010 | BioProduction |
| A-59 | A | Rasmus Wedberg | Simulation of proteins | JA | 7-2007 | 6-2010 | BioProduction |
| A-60 | A | Martin Dela Ellegaard | Thermodynamic properties and phase equilibria from fluctuation solution theory | JA | 2-2008 | 1-2011 | DTU |
| A-61 | A, B | Linfeng Yuan | Membrane assisted enzyme fractionation | GJ/JW | 2-2008 | 1-2011 | Novozymes |
| A-62 | B, D | Noor Asma Fazli Bin Abdul Samad | Control of process operations and monitoring of product qualities through hybrid multi-scale model-based analysis | RaG/GSI/ KVG | 1-2009 | 12-2011 | Malaysia |
| A-63 | A, B | Carlos Axel Díaz Tovar | Computer modelling of lipid processing | RaG/Bent | 3-2008 | 2-2011 | DTU/Alfa Laval |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | technology | Sarup | | | |
| A-66 | C | Alicia Román-Martinez | Design of intensified bioprocesses | RaG/JW | 7-2008 | 6-2011 | PROMEP, Mexico |
| A-68 | C, E | Chutima Swangkotchakorn | Optimization of tailor-made chemicals from renewable and non-renewable sources | RaG/JW/ JDG | 9-2008 | 8-2011 | DTU |
| A-69 | C | Albert Emili Cervera Padrell | Moving from batch towards continuous organic-chemical pharmaceutical production | KVG/SK/ RaG | 8-2008 | 7-2011 | DTU |
| A-70 | B, E | Martina Heitzig | Computer-aided modelling for efficient and innovative product-process engineering | RaG/GSI/ PGL | 12-2008 | 11-2011 | DTU |
| A-71 | C, E | Philip Lutze | Green chemistry based innovative process-operation synthesis and design | JW/RaG/ | 12-2008 | 11-2011 | DTU |
| A-72 | A, C | Azizul Azri Bin Mustaffa | Development and analysis of group-contribution$^{plus}$ models for property prediction of organic chemical systems | RaG/GK | 4-2009 | 3-2012 | Malaysia |
| **External PhD-Projects** | | | | | | | |
| **No.** | **Area** | **Personnel** | **Project Title** | **Supervisor** | **Start** | **End** | **Funding** |
| A-35 | C, E | Ana Carvalho | Sustainability analyses of chemical processes | RaG | 3-2006 | 2-2009 | Portugal |
| A-73 | B, C | Amnart Janthasurak | Methodology and algorithm for design and synthesis of reactive distillation process | RaG | 1-2009 | 7-2009 | Thailand |
| A-74 | A, C | Claudia Leonor Aguirre Céspedes | Group contribution-based estimation of pure component properties of ionic liquids | RaG | 2-2009 | 7-2009 | Chile |
| **Research Projects (not PhD)** | | | | | | | |
| **No.** | **Area** | **Personnel** | **Project Title** | **Supervisor** | **Start** | **End** | **Funding** |
| B-29 | | Romain Privat | Application of the GC-plus approach to PC-SAFT EOS and prediction of phase equilibria | RaG | 12-2008 | 9-2009 | NABIT/CAPEC |
| B-30 | | Jakob Kjøbsted Huusom | Model identification and optimal tuning for model predictive controllers | JBJ/NKP/ SBJ | 12-2008 | 11-2010 | IMM/KT |
| B-31 | | Ricardo Morales Rodriquez | Integrated modeling for simulation and design of novel enzymatic processes | GSI/KVG/ AM | 6-2009 | 5-2010 | FTP |
| **MSc-Projects** | | | | | | | |
| **No.** | **Area** | **Personnel** | **Project Title** | **Supervisor** | **Start** | **End** | **Funding** |
| C-45 | | Tolga Us | Functionality based abnormal situation | Morten | 8-2007 | 3-2008 | 45 points |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | management | Lind/SBJ/NJ | | | |
| C-46 Completed | B | Agnieszka Labrenz | Modelling of biofuel related transesterification reactions | RaG | 2-2007 | 7-2007 | 30 points |
| C-47 Completed | A, E | Sergey Maksimtchouk Nicolas Merigaud | CAPEC tool for group contribution model development | NJ | 3-2007 | 6-2007 | |
| C-48 Completed | A | Martin Christensen | Mixed solvent solubility – Data reduction | JA | 2-2007 | 4-2007 | 15 points |
| C-49 Completed | A | Martin Christensen | Mixed solvent solubility – Modeling | JA | 5-2007 | 12-2007 | 35 points |
| C-50 Completed | A, B | Kasper Andersen | Antibody production. Process analysis | JA | 2-2007 | 6-2007 | |
| C-51 Completed | C | Muhammad Shafique Bashir | Separation process design for azeotropic mixtures | RaG | 3-2007 | 6-2007 | 10 points |
| C-52 Completed | C | Muhammad Shafique Bashir | Solvent-based separations and organic synthesis | RaG | 9-2007 | 2-2008 | 30 points |
| C-53 Completed | A, B | Jes Schmidt-Petersen | Concentration and purification of enzymes by membrane filtration | GJ | 2-2007 | 6-2007 | 20 points |
| C-54 Completed | C | Shahid Ikram | Batch distillation design and analysis | RaG | 2-2007 | 6-2007 | 20 points |
| C-55 Completed | C, E | Naweed Al-Haque | Bio-refinery: Evaluation of process design alternatives | RaG | 2-2007 | 2-2008 | 40 points |
| C-56 Completed | C | Muhammad Riaz | Separation process design with ionic liquids | RaG | 7-2007 | 1-2008 | 30 points |
| C-57 Completed | D | Lago Freixeiro Díaz | Running in of experimental exercise for batch control | KHC/SBJ | 9-2007 | 6-2008 | 15 points + 7.5 |
| C-58 Completed | D | Diana Grandío Moirón | Running in of experimental exercise for batch control | KHC/SBJ | 9-2007 | 6-2008 | 15 points + 7.5 |
| C-59 Completed | A | Vijaya Kumar Kuchipudi | Structure/property relations. Data reduction, parameter variance and prediction intervals | JA | 8-2007 | 1-2008 | 30 points |
| C-60 Completed | F | Emilie Alletru | Separation of azeotropic mixtures | RaG | 11-2007 | 1-2008 | ERASMUS |
| C-62 Completed | A | Ashok Ratnam | Complex liquids | JA | 9-2007 | 4-2008 | |
| C-63 Completed | D | Mengzhe Wu | Towards simulation of cupola furnace for model based control | SBJ/JBJ | 9-2007 | 6-2008 | 35 points |
| C-64 Completed | C | Maria Abaigar Aranguren | Process design for ethanol production | RaG | 1-2008 | 5-2008 | 30 points |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C-65 Completed | E | João Terra | Analysis of a sustainable “model” refinery | RaG | 3-2008 | 7-2008 | 30 points ERASMUS |
| C-66 Completed | F | Adam El-Khamsi | Software development in ICAS | RaG | 4-2008 | 6-2008 | |
| C-67 Completed | B, D | Johan Bruun | Modelling and control of turbine with district heating | KHC | 9-2008 | 1-2009 | 30 points |
| C-68 Completed | B | Dres Foged Olsen | Modeling and simulation of single cell protein production | SBJ/JBJ | 9-2008 | 4-2009 | 30 points |
| C-69 Completed | C | Pramvit Nunthasanthi | Selection of material for polyethylene wax viscosity reduction | RaG | 9-2008 | 12-2008 | PPC, Thailand |
| C-70 Completed | F | Flora | Separation of azeotropic mixtures | RaG | 11-2008 | 1-2009 | ERASMUS (Pau, France) |
| C-71 | C | Pedro Ignacio Huertas Osta | Simulation, design and analysis of reaction separation process | RaG | 1-2009 | 6-2009 | 30 points |
| C-72 | A, B | Malene Kaab<br>Majken Boesgaard Graversen | Vacuum filtration of pectine solution | KHC | 2-2009 | 6-2009 | 20 points |
| C-73 | C | Nor Alafiza Yunus | Chemical product design | RaG | 5-2009 | 8-209 | UTM, Malaysia |
| C-74 | E | Gregory Guillotin | Sustainable process design: bioethanol production | RaG | 6-2009 | 9-2006 | ENSIC, Toulouse |
| C-75 | E | Marie Capron | Hazards and safety analysis | GSI | 6-2009 | 9-2009 | ENSIC, Toulouse |
| C-76 | C | Michele Mattei | Computer aided chemical product design | RaG | 10-2009 | 3-2010 | 30 point |

### 3.2 CAPEC research programs versus CAPEC co-workers

Table 3.2 provides an overview of the research programs and the CAPEC personnel involved with them

| **Research Programs** | **CAPEC coworkers & research activities** | | | | |
|---|---|---|---|---|---|
| | **Faculty**[1] | **Post-Docs**[2] | **PhD-students**[2] | **MSc-students** | **Others**[3] |
| **A: Property & Phenomena Modelling** | **JA**; GJ; RaG | ***RP;*** (*RC)* | (SPB; HEG); ***KAC***; ***RAW; ELC; LYF; MEC; AZM*** | ***(A Ratnam), P Huertas*** | **C Aguirre** |
| **B: Product & Process Modelling** | **RaG**; JA; GJ; (SBJ);GSI | ***RMR*** | (RMR; JAR); ***RS; MAL; ELC; OAP; LYF; NAS; ARM; MAT; ADI*** | ***P Huertas*** | **A Carvalho; A Janthasurak** |
| **C: Synthesis, Design & Analysis** | **RaG**; JA; GJ; (SBJ); GSI | | (PTM; JAR) ***KAC; MAL; ELC ; MKA; OAP; ARM; CHS; AZM; ADI; ACP; PIL*** | ***(M A Aranguren)*** | **A Janthasurak;** *N A Yunus; (P Nunthasanthi)* |
| **D: Control, Operation & Monitoring** | **(SBJ); GSI**; KHC; RaG | ***JKH*** | (JKH); ***RS; MKA; OAP; NAS*** | ***(D F Olsen), (JB), (M Wu), (D G Moiron), (L F Diaz)*** | |
| **E: Process & Tools Integration** | **RaG**; GJ, SBJ; GSI | | (PTM; RMR); ***MAL; MKA; CHS; MAT; PIL*** | ***(J Terra)*** | **A Carvalho** |
| **F: Databases & Numerical Methods** | **JA**; RaG | | | | *(A El-Khamsi); (Flore)* |
| **Currently active** | **4 + 1 + 1** | **3** | **17** | **1** | **3** |

1: Research area coordinators are indicated in bold; 2: New coworkers since June 2008 are indicated in bold-italic; 3: These are external PhD-students (bold) and visiting students (italic) and/or short-term visiting researchers

## 3.3 PhD-Research Project Overview

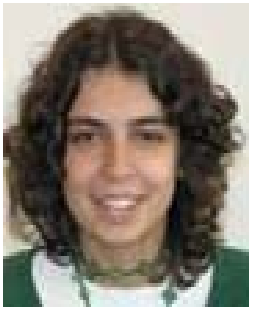
**Merlin Alvarado-Morales** (MAL)
Supervisors: RaG, KVG, JW
Started: 01-04-2007
Finish: 31-03-2010

*Research area: Process modeling, synthesis, design*

***Process-product Synthesis, Design and Analysis through the Group-Contribution Approach***

The core idea is to apply the group contribution approach for property estimation to the synthesis, design and analysis of various types of products and their corresponding processes, with groups (or atoms, etc.) representing units, bonds representing streams, rules for molecule feasibility representing flowsheet feasibility and sum of group contributions representing the performance of the flowsheet. The main idea behind of the GC-concept is that similar structural descriptors (process groups and molecular groups) are used to represent the molecular and process flowsheet structures and to predict their behaviour through a set of regressed group contributions. The earlier work has established the GC-concept through proof of concept examples and processes from the chemical industry. Therefore, the objective of this PhD project is to develop simple, fast yet reliable methods for synthesis, design and analysis of various types of products and their corresponding processes related to the chemical, food and bio industries.

**Ana Isabel Carvalho** (AC)
Supervisors: H. Matos, RaG
Started: 01-03-2006
Finsh: 01-02-2010



*Research area: Process design, sustainability, integration*

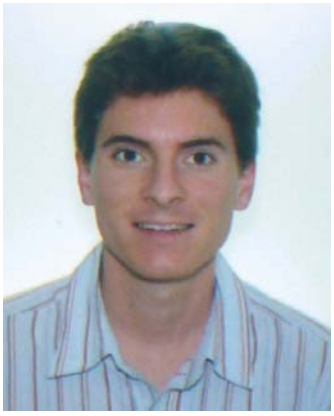
***Systematic methodology for design of sustainable chemical processes***

A systematic methodology for process analysis and screening, which is able to generate new sustainable process design alternatives, has been developed. This methodology locates the operational, environmental and safety bottlenecks inherent in the process through a set of mass and energy indicators and suggests new design alternatives that improve the identified process bottlenecks. Based on this methodology, a software called Sustain-Pro has been developed. Sustain-pro as well as the indicator based methodology has been tested for several continuous processes (such as the well-known HDA-process, VCM process and the Ammonia process) as well as batch processes (wash water in laundry; insulin production). Current work involves integrating Sustain-Pro with an external software for waste minimization and development of more case studies from industries.

**Albert Emili Cervera Padrell** (ACP)
Supervisors: KVG, SK, RaG
Started: 01-08-2008
Finish: 31–7-2011

***Moving from batch towards continuous organic-chemical pharmaceutical production***

Organic synthesis based pharmaceuticals have traditionally been produced in batch reactors, and it is custom to tailor the synthetic routes to work well in these reactors instead of using reactor set ups designed to handle the relevant chemistry. This results in time-consuming production processes that often need expensive storage of reaction intermediates as well. As such, batch production also implies that the full benefits of the Process Analytical Technology (PAT) initiative of the FDA



**Martin Dela Ellegaard** (MEC)
Supervisors: JA
Started: 01-02-2008
Finish: 31-01-2011

**ELISA CONTE** (ELC)
Supervisors: RaG
Started: 01-07-2007
Finish: 30-06-2010

*Research area: Property modeling, product design*

**Carlos Axel Díaz Tovar** (ADI)
Supervisors: RaG; Bent Sarup (Alfa Laval)

cannot be realized in the pharmaceutical production process. In contrast, a continuous production environment may potentially lead to improved safety against e.g. runaway reactions, higher productivity and reduced costs, and reduction or elimination of stocks. The aim of this PhD project is to develop continuous operation units optimized for a certain type of reaction or separation process, ideally preserving flexibility. Such approach should yield a methodology and a set of toolboxes applicable to similar design problems.

*Research area: Process modeling, synthesis, design*

***Thermodynamic properties and phase equilibria from fluctuation solution theory***

Motivation of this project is the accurate solubility estimates important in downstream processes; optimal solvent selection; based on behavior of solids in mixed solvents that is difficult to predict as extrapolation between solvents is not straightforward.
Another objective is the application of the statistical mechanical fluctuation solution theory to gas solubilities in ionic liquids from a group contribution approach.

*Research area: Property modeling*

***Innovation in Integrated Chemical product-process Design: Development through a Model-based Systems Approach***

Consumer-oriented chemical products are complex products (formulations, mixtures, emulsions, etc.) which have to show the right properties in order to meet the consumer needs. The role of chemical product and process design is to find a candidate product that exhibits the targeted behavior and a process that can manufacture it for the specified qualities. The aim of this project is to develop a *Virtual* Product–Process Design Lab through which innovative solutions for product and process design can be obtained. Through the *Virtual* Lab it is possible to rapidly search and test a large number of candidates and identify a few promising ones that can be further examined through appropriate experiments. In this way, computer aided methods and tools are employed for the initial search while the experimental resources are reserved for testing a few alternatives among which the optimal product is likely to be found. Design of various types of formulated products such as shampoo, sunscreen lotion, hair spray, etc., from the everyday life are being studied.

***Computer Aided Modeling of Lipid Processing Technology***

The production of edible fats and oils, like many other

Started: 01-05-2008
Finish: 30-04-2011

**Mohd. Kamaruddin bin Abd. Hamid** (MKA)
Supervisors: RaG, GSI
Started: 01-07-2007
Finish: 30-06-2010

*Research area: Integration of process design & control*

**Martina Heitzig** (MAT)
Supervisors: RaG, PGL, GSI
Started: 01-12-2008
Finish: 30-11-2011

chemical processes, involves a wide range of processing steps, from crude edible oil (vegetable) production to the final product. However, unlike the chemical processes, the state of the art in process modeling and simulation has only to a very limited extent penetrated this industry, due to the complex nature of the lipid systems involved. Modeling and validation of physical properties of the most representative chemical species and their mixtures occurring on the edible oil industry, as well as optimization of the associated unit operations and process sections are the main objectives of this PhD project.

*Research area: Property-process modeling, process design*

***Integration of Modelling, Design and Control for Efficient Operation of Chemical Processes***

In classical process development, design and control decisions are made sequentially with the common aim of ensuring profitable and robust operable process. As a result, controller tuning and optimization is limited by process dynamics already fixed in the design phase. At the same time it does not guarantee robustness under uncertainty and often fails to describe actual process dynamics. In order to achieve the best profitable and robust operable process, it is necessary to consider process design and control decision simultaneously. Recently, several methodologies have been developed for the integrated process design and control (IPDC). In spite of their progress in IPDC field, the available methodologies still offer insufficient insight to the problems. In practice, a systematic tool that can assist in deciding the best solution for IPDC problems is needed. Therefore, the objective of this research is to develop a systematic model-based methodology which is capable of designing chemical processes that will have the best performances in terms of design, control and economic effectively and in an integrated manner.

***Computer-aided modelling for efficient and innovative product-process engineering***

Computer-aided modelling plays a role of increasing importance in almost all industries related to chemical and biochemical engineering due to its ability to reduce the number of cost-intensive, time-consuming and resource-demanding experiments but also because it has the potential to deliver truly innovative solutions that might not necessarily be obtained by conventional trial-and-error approaches. The core perquisite however, is to provide predictive models that are able to represent the investigated systems to the degree of detail required for the special application. The objective of this project is to systematize the process of model development and increase its efficiency by developing a computer-aided modelling framework that provides the required work- and

*Research area: Computer aided modeling*

data-flows to solve a large variety of different modelling problems. The framework guides the user through the work-flow, combines the required tools and database connections where needed and offers expertise the user might not have. The computer aided framework supports multi-scale modelling and the archiving and re-use of models.

**Philip Lutze** (PIL)
Supervisors: JMW, RaG
Started: 01-12-2008
Finish: 30-11-2011

*Research area: Synthesis; process intensification*

***Development of a systematic synthesis methodology for achieving process intensification***

The chemical, biochemical and pharmaceutical industry is facing new challenges which need improvements in whole processes. One option to achieve these improvements is through process intensification, which can be defined as an engineering strategy to achieve improvements in processing/operation through synthesis/design of the process and/or design of new equipments. However, implementing process intensification into industry is still not simple and systematic. Therefore the objective of this work is to develop a systematic synthesis methodology to achieve process intensification. The method is based on solid understanding of the underlying principles that promote intensification and will generate possible intensified innovative process alternatives which are validated through an indicator metrics. The developed methodology will be tested and verified with case studies from the chemical, biochemical and pharmaceutical sectors.

**Azizul Azri Bin Mustafa** (AZM)
Supervisors: RaG, GK
Started: 01-4-2009
Finish: 31-03- 2012

*Research area: Property modeling; process-product design*

***Development and Analysis of GC$^{Plus}$ Models for Property Prediction of Organic Chemical Systems***

The prediction of properties in chemical process and product design is important and the implementation of a property model that can estimate the needed properties efficiently and reliably is the most wanted solution. However, due to the increased complexity of chemical molecular structures, wider range of chemicals and accuracy, further development of the current prediction methods and techniques as well as development and analysis of new models are necessary. In accordance with that, recently a new combined group-contribution and atom connectivity approach that is able to extend the application range of property models has been developed to estimate the properties of pure components as well as mixtures. It combines group contribution theory and molecular descriptors theory using the Group-Contribution$^{Plus}$ (GC$^{Plus}$) approach. The objectives of this work will be to further develop other versions of the UNIFAC models and to complete the UNIFAC Dortmund parameter table. In addition, the performances of the GC$^{Plus}$ approach various equilibrium systems such as VLE, LLE, SLE and others will be evaluated. The prediction accuracy in terms of uncertainties in these systems needs also to be analyzed. Finally, the hybrid models

developed will be applied in innovative chemical product synthesis and design.

**Oscar A Prado-Rubio**(OAP)
Supervisors: GJ, (SBJ)
Started: 01-06-2007
Finish: 31-05-2010

*Research area: Separation (membrane); design, modelling*

***Modelling and Optimization of Integrated Bioreactor and Membrane Separation Processes***

The fermentation of Lactic acid by Lactic Acid Bacteria is normally impaired by product inhibition like many other fermentation processes at a certain concentration level of the product or one of the bi-products. Therefore, continuous removal of Lactate from the fermenter will result in a higher productivity and product yield. Integrating separation and fermentation will also enable operation at higher cell densities, thereby providing additional enhanced productivity potential. The objective of this project is to derive, validate and investigate a dynamic model for an integrated bioreactor and electrically driven membrane separation processes. The purpose of this model is to optimize the design and operation of lactic acid fermentation according to different objectives. Finally, it is aimed to evaluate the influence of different process scales.

**Jamal El Bashir Ali Rashed** (JAR)
Supervisors: RaG
Started: 01-01-2006
Finish: 26-06-2009

*Research area: Retrofit process synthesis and design*

***Model-based retrofit design and analysis of petrochemical processes***

Technological, economical and new environmental regulation changes have an important impact on the petrochemical processing industry. As a result, many of the existing production processes require constant improvements through retrofitting that are available by generation of new alternatives to the process that exhibit improvements on design parameters such as operability, cost, waste reduction and environmental impact. This project presents the development of a systematic methodology plus its associated algorithms for generate and screen feasible retrofit process alternatives, to produce the same products from the same raw materials and from them, to identify the more sustainable ones. The methodology is organized in three stages: 1. targeted process analysis (process flowsheet is analyzed in order to identify the design/operational weak points); 2. reverse process synthesis and design (identification of feasible process options and match of the target with design alternatives); and 3. final selection and verification (comparison of performances of feasible process alternatives for final selection). Several case studies have been solved.

**Alicia Román Martínez** (ARM)
Supervisors: RaG, JW
Started: 01-08-2008
Finish: 31-07-2011

***Design of Intensified Bioprocesses***

The objective is to develop a systematic model-based generic methodology for design and development of intensified bioprocesses, considering the integration of chemical and

enzymatic reactions (one-pot synthesis) and downstream processing stages (*in-situ* product removal, ISPR); to provide process improvements by increasing yield, reducing processing time and reducing costs. This methodology also considers technical and economical aspects, to achieve the goal of rational process development that will maximize the product yield, selectivity, productivity, biocatalyst stability as well as profitability, while trying to minimize energy requirements by employing fewer processing steps and higher yields in each step. Consequently, different routes of synthesis are generated and evaluated an optimal bioprocess configuration is selected and validated.

*Research area: Bio-process modeling, synthesis, design*

**Noor Asma Fazli Abdul Samad** (NAS)
Supervisors: RaG, KVG, GSI
Started: 01-01-2009
Finish: 31-12-2011

*Research area: Process modeling, product quality control*

***Control of process operations and monitoring of product qualities through hybrid multiscale model-based analysis***

Modeling of chemical/biochemical processes is a common tool in process technology. Accurate models of the underlying processes are essential for design, optimization and control. However, in many situations of industrial interest detailed models are not available due to insufficient understanding of the underlying phenomena. Also, the properties of structured chemical products need to be defined at the microscopic level while its end-use properties are defined at the macroscopic level. This lack of available models and corresponding parameters may be dealt with through the employment of hybrid multiscale modeling strategies. Meanwhile model based techniques, combined with available data/knowledge can make a significant contribution in process-product design and development through systematic and efficient work-flow and data-flow for the various associated sub-problems. Therefore the main tasks of the PhD-project would be to develop a modeling framework for generation and analysis of hybrid multiscale models and to build a model-based approach for process-product monitoring, control and analysis. Case study involving crystallization process will be considered as the first process-product in this work.

**Kavitha Chelakara Satyanarayana** (KAC)
Supervisors: JA, RAG
Started:01-06-2006
Finish: 31-05-2009

***Molecular design using grid technology***

A multiscale modelling approach is taken into consideration for designing polymer based products starting from a basic repeat unit design to the final polymeric chain design. The CAMD algorithm uses some fragments to design a repeat unit. Using the macro scale approach, the fragments used for the repeat unit design are the groups defined by Marrero/Gani (MG) and the property prediction models are based on MG group contribution approach. As there is a limitation on the availability of extensive experimental values of polymer properties, one cannot expect the entire group table without missing parameter entities. At times, there can be molecular structures that cannot be totally represented by groups in the

specified group contribution methods. A meso scale approach is therefore considered at this point where an Atom-Connectivity method is applied. The missing group and/or the missing group contributions for a property are determined using the atom-connectivity models. The integration of group contribution and atom-connectivity index model is termed as group contribution plus model (GC+) and this approach has now been extended for the prediction of polymer properties using the basic repeat units. These GC+ models are implemented in CAMD algorithm. A number of case studies have been solved and the method is being further extended into the micro-scale to consider the arrangement of the identified polymer repeat units.

*Research area: Polymer property modeling, product design*

**Ravendra Singh** (RS)
Supervisors: RaG, KVG
Started: 01-09-2006
Finish: 31-09-2009

*Research area: Process analytical technology; modelling*

***Model-based computer aided framework for design of process monitoring and analysis systems***

The objective of this project is to develop a systematic methodology plus accompanying software for design of process monitoring and analysis systems. The design methodology and corresponding software (ICAS-PAT) for design of PAT (Process Analytical Technology) system has been developed. Two supporting tools (knowledge base & model library) needed by ICAS-PAT have also been developed. The supporting tool knowledge base consists of two sections. The first section of the knowledge base summarizes the process knowledge (type of processes, and corresponding process variables, etc.) while the second section of the knowledge base consist of the knowledge of measurement methods and tools (type of variables, available monitoring techniques, accuracy, operating range, response time, cost etc.). The model library contains a set of mathematical models for different types of unit processes, sensors and controllers. The software ICAS-PAT has potential application in pharmaceutical, bio and food industries. Three case studies involving a pharmaceutical tablet manufacturing process, Insulin production process and cheese manufacturing process has been developed.

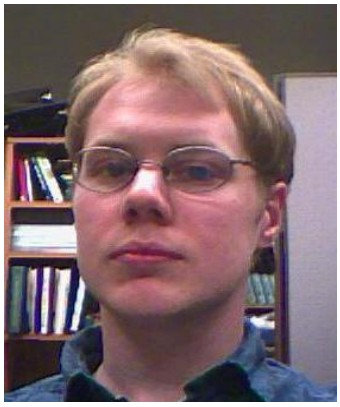
**Chutima Swangkotchakorn** (CHS)
Supervisors: RaG, JW, JDG
Started: 01-09- 2008
Finish: 31-08-2011

***Optimization of tailor-made chemicals from renewable and non-renewable sources***

In the future, the chemical industry will need to be based on the conversion of renewable material, such as biomass, and in particular, lignocellulosic biomass. In order to meet the world's needs for industrial chemicals and liquid fuels, while minimizing the environmental impact, the economic and societal benefits would need to be maximized through the use of a new strategy. The objective of this PhD project is to develop a model biorefinery by matching a set of biomaterial feedstocks to an optimal set of end-point products (chemicals

and fuels) through a range of sustainable processing routes. Economic and environment impacts will be minimized through the optimal use of renewable and non-renewable feedstocks.

*Research area: Biorefinery modeling, optimization*



**Rasmus Wedberg** (RAW)
Supervisors: JA
Started: 01-11-2007
Finish: 31-10-2010

***Simulation of Proteins***

In this project, molecular modelling and simulation is applied to study solvent effects on lipase B from *Candida Antarctica*, a catalyst commonly applied for a large number of reactions, *e.g.* transesterifications. The enzyme, representative substrates and activated complexes will be simulated in various solvents using molecular dynamics simulations and possibly also QM/MM methods. A number of calculations of properties that can be correlated with the activity, for example, free energy differences and conformational flexibility near the active site, will be carried out. The aim is to make qualitative statements about the effects the solvent will have on the activity. The results will be verified by kinetics measurements performed by our collaborators.

*Research area: Molecular modelling*

**Linfeng Yuan** (LFY)
Supervisors: GJ, JW
Started: 15-03-2009
Finish: 01-04-2011

***Membrane Assisted Enzyme Fractionation***

Large-scale economic purification of enzymes with high selectivity is becoming increasingly an important problem for the biotechnology industry. Generally, separation of the desired enzyme from other enzymes produced by the cell is attempted using a combination of different chromatography techniques in order to achieve adequate purity or using membrane filtration. However, membrane filtration has low selectivity because of different enzyme with similar size in the complex feeds while chromatography is expensive. The aims of this project are to develop a suitable membrane fractionation process and to assess the economics of such membrane processes for industrial scale production of relevant applications such as pharmaceutical and dairy enzyme production. If an efficient process is developed, then pilot up-scaling of the membrane fractionation process will be considered.

*Research area: Membrane assisted separation (enzyme purification)*

## 3.4 External PhD-students (projects)

### *3.4.1 Computer aided design of ionic liquids (Claudia Leonor Aguirre Cespedes, University of Antofagasta, Chile)*

Ionic liquids (ILs), as green solvents, have been extensively studied due to their tempting properties such as negligible vapor pressure, large liquids range, high thermal stability, high ionic conductivity, large electrochemical window, and ability to solvate compounds of widely varying polarity. Using ILs is one of the goals of green chemistry because it has been claimed they create a cleaner and more sustainable chemistry and are therefore receiving an increased interest as environmental friendly solvents for many synthetic and catalytic processes. An intriguing characteristic is to tune the physical-chemical properties by suitable choice of cations and anions. Therefore, ILs have been recognized as "designer-solvents".

To optimize the use of ILs and design of desirable tailored ILs, knowledge of the physical and chemical properties of ILs; and the ability to estimate them are essentially important.
From the industrial standpoint, a fundamental understanding of the chemical and physical properties of ILs should be known before its industrial application.

The objectives of this PhD-project is to create a database with all ionic liquids that can be formed through the available groups, predict the properties of these ILs, and extend the group parameter tables to predict properties of those ionic liquids that could not be handled because of the missing group parameters. Due to the large number of potential ionic liquids that can be already formed, it is expected that this database can be used to identify and select ionic liquids with desired (target) properties, as well as to find new properties to be modelled that will be necessary for a wider range of applications of ionic liquids. In this way, the created database of existing and new ILs will be equipped with a search engine to quickly identify the needed IL, if it exists.

### *3.4.2 Methodology and algorithm for design and synthesis of reactive distillation columns (Amnart Janthasurak, Chulalongkorn University – SCG Chemicals, Bangkok, Thailand)*

Reactive distillation one of the most important applications of the integrated reaction and separation concept, is a combination of chemical reaction and separation via distillation (two operations within a single apparatus). Due to the demand for more efficient processes in today's chemical industry, reactive distillation provides promising alternatives to conventional sequential operations-the reaction unit following by the distillation train, because it offers the main advantages of reducing the equipment costs, improved heat efficiency and enhanced reactant conversion and selectivity. Nowadays, the design of reactive distillation based on the laboratory and pilot plant experiments is expensive and time consuming. Therefore, it is not economically feasible to test many design alternatives through experiments. Model-based design coupled with experimental verification on the final design is a promising option. One very useful method for reactive distillation column is the element based approach coupled with the driving force diagram. The main idea here is that "the highest driving force refers to the minimum energy consumption". Also the application of element based approach can reduce the dimension of the system (the number of elements is less or equal to the number of components). Nevertheless, the application of element based driving force diagram still has the drawback that it can handle only two dimension systems (two elements). For the method to be generic, multi-element systems need to be handled.

The objective of this work is to develop a methodology for design and analysis of reactive distillation columns for multicomponent reactive systems. The concept of driving-force and reverse design approach will be combined to determine near-optimal designs with respect to energy consumption, waste and cost. Hengstebeck's procedure for reduction of multicomponent systems to binary systems will be adapted to "elements" so that multi-element reactive systems can also be reduced to binary element systems. From the binary reactive element driving force and vapor-liquid phase (reactive) diagrams, the already established methods for distillation design will be applied. Here, the driving-force diagram will first be used to identify the location of the maximum driving force (according to the driving force concept, larger driving force implies better separation, less waste, less energy consumption and therefore, lower cost). The reverse approach helps to determine the design of the distillation column that matches the target driving force. Once the reactive distillation design has been obtained, it will be validated with rigorous reactive distillation models and then, if feasible, through experiments.

### 3.5 Post-Doctoral Research Project Overview

**Jakob K Huusom** (JKH)
Supervisors: RAG, SBJ, GSI (KT) & NKP, JBJ (IMM)
Started: 1-12-2008
Finish: 30-11-2010

***Model Identification and Optimal Tuning for Model Predictive Controllers***

In this project we will investigate methods for shortening commissioning times and improving quality in model predictive control applications. The contributions of this project will stem from addressing the problems related to commissioning and maintenance of MPC controllers from several angles. First, the use of process models which are tailored specifically for use with MPC and identification methods that are well suited for use in industrial settings are to be investigated. Second, control performance will be improved through application of several tuning methods to the controller modules. These methods are used for selection of optimal tuning parameters in the controller, estimation of noise statistics and identification of disturbances.

**Romain PRIVAT** (ROP)
Supervisor: RaG
Started: 01-12-2008
Finish: 30-11-2009

*Application of the GC-plus approach to PC-SAFT EOS and prediction of phase equilibria*

This project is aimed at extending the application range of the PC-SAFT equation of state. The description of fluid mixtures involves the knowledge of three parameters ($m$,$\sigma$, $\varepsilon/k$) per component in the mixture. First time, we addressed the calculation of these parameters from pure component VLE data for nearly 1000 molecules. In the next step, a group contribution (GC) method has been developed to predict the same 3 parameters. Quite satisfactory results have been obtained.

In particular, thanks to this GC method, the PC-SAFT parameters of polymers can be estimated. Here again, accurate results have been obtained. The next step was to employ a connectivity index (CI) method to estimate the same 3 parameters. With this option, it is possible to predict the necessary parameters when experimental data or group contributions are not available. With the pure component parameters for the PC-SAFT available, predictions of phase equilibria for multicomponent mixtures can be made.

**Ricardo Morales Rodriguez**
(RMR)
Supervisors: GSI
Started: 01/06/2009
Finish: 31/05/2010

***Integrated modelling for simulation and design of novel enzymatic processes***

Currently the development and transfer of the novel enzymatic processes including production of biofuels, prebiotics and the like from the proof-of-concept at bench-scale to industrial scale are mainly done empirically and based on experiences from conventional one-pot conversion processes. This approach is rather inefficient and costly and may not even offer the most optimal and sustainable solutions. To resolve these challenges, this project aims to introduce a more rational model-based simulation framework for enzyme process design using:

- Model simulations to facilitate the rational development and boost innovative designs of new enzyme processes.
- Cutting edge techniques in system analysis, simulation and optimization sciences.

Ultimately, the project aims to move the practice from empirical to a more efficient and advanced simulation and prediction based design approach.

## 4. CAPEC Software

Development of CAPEC software is closely related to the CAPEC research projects. Since a majority of CAPEC research projects deal with the use of computers to solve process/product engineering problems, the theories and algorithms developed in the research projects are validated through these computer programs. Among these, the computer programs that have a general appeal with respect to their application and do not have any restrictions imposed by a consortium member company, are collected and distributed as part of the CAPEC software. CAPEC software is not a commercial software and are distributed exclusively only to the CAPEC industrial consortium member companies. A special version is distributed at a nominal price for educational purposes.

The objective of the CAPEC software is to promote the use of computer aided methods and tools developed by CAPEC in the solution of current and future process/product engineering problems. The CAPEC software consists of the following:

- Integrated Computer Aided System – ICAS
- EXCEL based macros (ProPred, CAPECDB Manager)
- Continuous Time Stochastic Modeling – CTSM
- UNIFAC-Utility (group definitions, VLE database, etc.)
- Grid of Linear Models – GoLM
- Special Software (ICAS-PAT, SustainPro, *v*PPD-*Lab*)
- PC-SAFT software package (trial version)
- SMSWIN – A tool for properties and phase equilibrium calculations, especially suitable for solid-liquid systems (compliments with the features in ICAS)

### 4.1 Integrated Computer Aided System – ICAS 12.0

ICAS combines computer-aided tools for modelling, simulation (including property prediction), synthesis/design, control and analysis into a single integrated system. These tools are present in ICAS as toolboxes. During the solution of a problem, the user may move from one toolbox to another to solve problems requiring more than one tool. For example, in process synthesis, one option is to define the feed stream, then analyse the mixture (analysis and utility toolbox), then generate a flowsheet (synthesis toolbox), then optimise the flowsheet (design toolbox), and finally verify the design (analysis toolbox). From any toolbox it is possible to invoke the simulation engine to perform steady state and/or dynamic simulation for batch and/or continuous process operations. From the synthesis toolbox, it is possible to invoke the solvent design tool (in design toolbox) if a solvent is needed for a specific separation task. There is also a utility toolbox, which determines properties, phase diagrams, etc., which can be used by the other toolboxes or by the user to analyze the behaviour of the specified system. “ICAS documentations” provides information on installation of ICAS, tutorials at basic and advanced levels and other useful information such as a list of dll-files copied during installation and new features of the latest version of ICAS. Figure 4.1 highlights the idea of integration and the advantages that can be obtained through this integration.

In ICAS 12.0, new features have been added to the following tools: ProPred (pure component property prediction), MoT (modelling toolbox), ProCamd (computer aided molecular design), and the CAPEC-database. The EXCEL based macros (ProPred and

CAPECDB manager) have been updated with new features and corresponding manuals. The CAPECDB manager also includes an azeotropic data collection and analysis feature. In addition, three special software (EXCEL based): Sustain-Pro, ICAS-PAT and the Virtual PPD-lab (*v*PPDL) have been revised and improved. Each of these software, use a number of ICAS tools and models generated through MoT. For a list of ICAS tools, see ICAS Documentation or the ICAS poster. A number of new properties for organic chemicals as well as polymer repeat units have been added to ProPred. In ProCAMD, it is now possible to design the polymer repeat units as well as check for target properties of generated structures through ProPred.

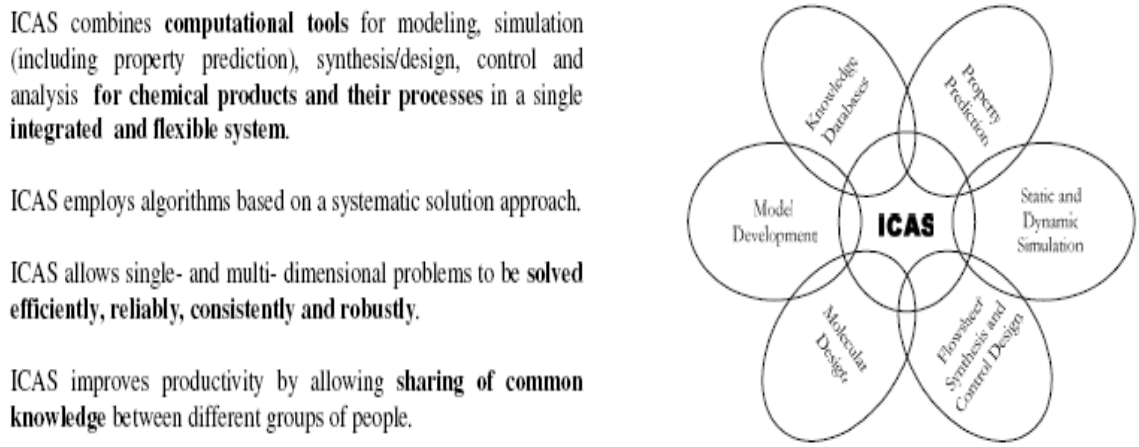



Figure 4.1: The idea of integration within ICAS

In general, ICAS 12.0 has become a much more robust and reliable version of ICAS with a wider application range. Finally, new additions to ICAS documents related to ProCAFD and Batch-Dis can be found after installation of ICAS under the examples-directory. New versions of manuals for the following tools in ICAS are also available - ProPred, MoT, SoluCalc and ProCamd. After installation of ICAS, users will find a number of worked out examples given in the "examples" and "tutorials" directories. Figure 4.2 highlights the new features in ICAS 12.0 while Fig. 4.3 highlights the work-flow in the implementation of a model (starting from transferring the published model equations to MoT and ending with a COM-object that can be executed from different external software).

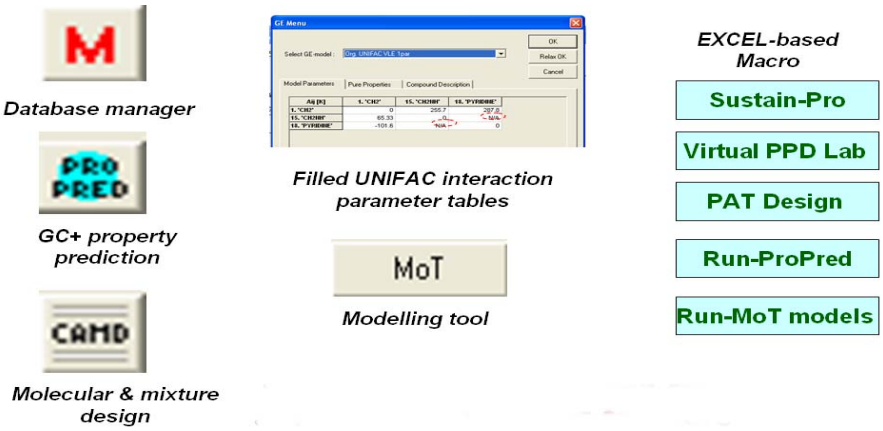



Figure 4.2: Highlight of new features in ICAS 12.0

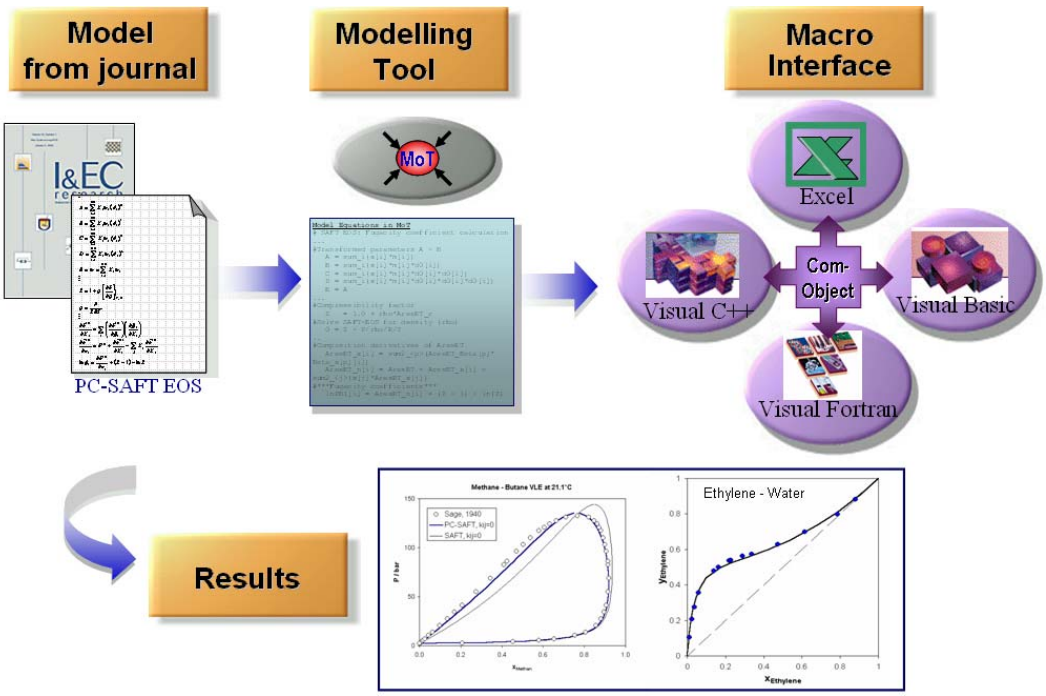



Figure 4.3: COM-object generation through MoT and use in external software

## 4.2 EXCEL based macros (ProPred, CAPECDB Manager)

Two EXCEL based software has been developed to further facilitate the use of ICAS-ProPred and the CAPEC-database. EXCEL-ProPred, the user opens the EXCEL macro and then performs different property calculations through ProPred. Here, the EXCEL spreadsheets become the working area and ProPred is the property calculator.

In the CAPECDB Manager, the EXCEL macro helps the user in the search for data available in the CAPEC database. A new feature to this database is the availability of azeotropic data.

## 4.3 Continuous Time Stochastic Modeling - CTSM

Continuous Time Stochastic Modelling means semi-physical modelling of dynamic systems based on stochastic differential equations. Stochastic differential equations contain a diffusion term to account for random effects, but are otherwise structurally similar to ordinary differential equations. This means that conventional modelling based on the principles of physics can be applied to set up the model structure.

With the model structure given, CTSM provides methods for estimating any unknown parameters of the model from time series data, including the parameters of the diffusion term. These methods are able to handle both linear and nonlinear models, and the program also provides great flexibility with respect to the data that can be used, *e.g.* by allowing varying sample times, missing observations and occasional outliers.

The methods implemented in CTSM are a *maximum likelihood* (ML) method and a *maximum a posteriori* (MAP) method. With both methods the program provides the ability to use several independent data files, just as it is possible to estimate initial conditions, if these are unknown. The ML and MAP methods are both sound statistically based

estimation methods, which means that once the parameters have been estimated, statistical tests can easily be performed to test the validity of the corresponding model. Some such test features are included in CTSM and others will be included at a later stage. The new version of CTSM is 2.2, which has a graphical user interface for setting up models, estimating parameters and generating validation data. This new version has an improved solution of the stochastic differential equations by using a stiff numerical integration routine. Furthermore the flexibility in applying the uncovering of too simply modelled functionalities has been increased, among others by enabling much simpler modification of the models. These modifications are needed for revealing unknown functionalities from experimental data.

## 4.4 UNIFAC-Utility

*KT-UNIFAC*-utility is a program that helps the user to check the consistency of UNIFAC groups, their parameter values and the representation of the molecules with the UNIFAC groups. For a specified mixture, the program determines the UNIFAC group information and passes the relevant data to ICAS for use in TML and other tools.

## 4.5 Special ICAS-based software (ICAS-PAT, SustainPro, vPPD-lab)

### *4.5.1 ICAS-PAT*

ICAS-PAT is an EXCEL based software that designs and/or analyzes a process monitoring system, given the process information. It has a built-in knowledge base of information about process operations, the variables that need to be measured, the variables that need to be monitored and the equipments that could be used. It also has a library of models that may be needed to supplement the data available for the process under investigation. The library models are run through ICAS-MoT. The EXCEL macro guides the user through an established work-flow based on the systematic methodology developed by Singh et al. (see PEC08-05). A manual and several solved case studies are available. Figure 4.4a highlights the main features of ICAS-PAT.

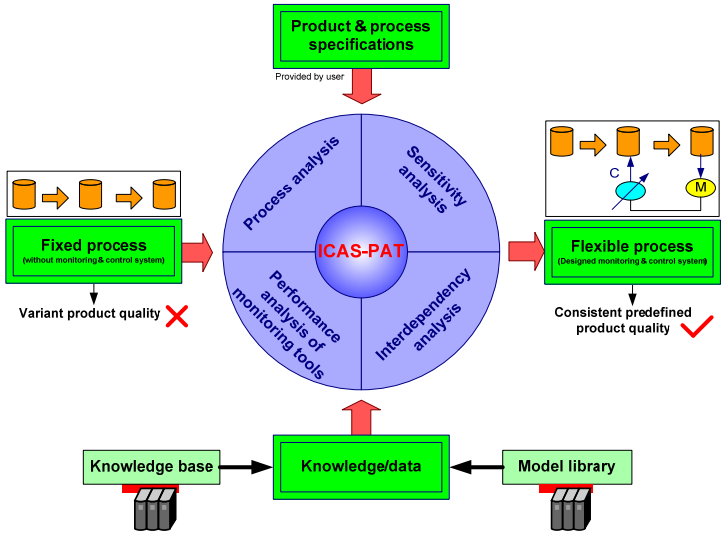



Figure 4.4a: Overview of the main features of ICAS-PAT.

### *4.5.2 SustainPro*

*SustainPro* is an *EXCEL* based software, which provides options for retrofit analysis and performance analysis of a given process. As highlighted in Fig 4.4b, the inputs to *SustainPro* are the mass and the energy balance data that can be collected either from the plant or from process simulations. To perform the retrofit analysis, *SustainPro* also requires as input, several cost related data (the prices for utilities, the prices for chemicals, etc.). *SustainPro* is able to read the mass and the energy balance from an *EXCEL* file generated by a commercial simulator. The EXCEL interface guides the user through the steps of the work-flow (solution steps). After applying all the steps *SustainPro* gives as output for the retrofit analysis, a new design alternative suggestion for improving the process being investigated. When the software is used for performance analysis, the output provides the calculated values of the sustainability metrics and the safety indices. As it can be seen from Fig 4.4b, the two options can be combined, which means that they complement each other. After applying the retrofit analysis, the performance analysis is performed and compared with the base case design.

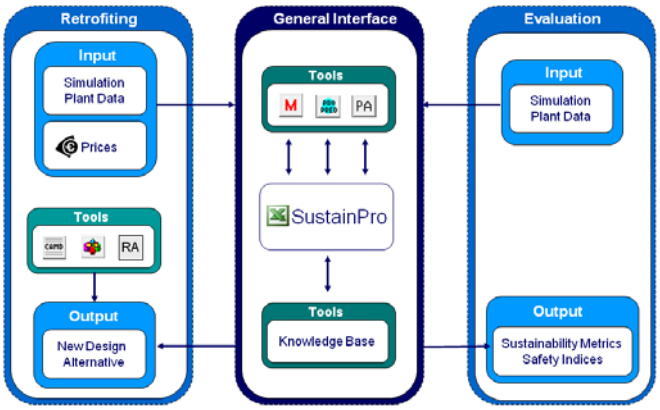



Figure 4.4b: Overview of the main features of SustainPro

### *4.5.3 Virtual Product-Process Design Lab*

The idea behind the virtual product-process design lab is the following: instead of doing the experiments needed to search for a product and its process to manufacture it, the engineer/scientist performs *virtual* experiments, through the *v*PPD-lab software. The software therefore contains a large knowledge base of data (of chemicals, of solvents, of plants, of microcapsule devices, etc.); a large collection of models (models for property prediction, models for controlled release, models for mixing, etc.); of design algorithms (methods for formulation design, methods for molecule design, methods for polymer design, methods for process flowsheet synthesis, etc); other tools (property prediction software; model generation software; equipment design software; design of experiments software, etc.). All of the above are organized through a framework for efficient management of the complexity. Figure 4.4c gives an overview of the main features of the *v*PPD-lab software, which has been used in the design and evaluation of the controlled release of a drug active ingredient (codeine) through a polymeric microcapsule. In the first step the problem is defined (identity of the active ingredient; the desired controlled release parameters, etc., are given in the "documentation" box of *v*PPD-lab). In the second step the selection of the application source (codeine released into the body), the primary properties of solvent and the polymer (needed by the controlled release model) is made (if the user is

unable to provide this information, methods for solvent design and polymer design are used to generate a list of candidates to select from). In the next step the selection and calculation of the functional properties needed to evaluate the controlled release design is made (if models are not available, the modelling software helps to generate new models). In the next steps, the product performance model is used to predict the product behaviour. If the desired (target) performance is matched, then the last step of verifying the product performance through experiments is performed. If the target is not matched, it is possible to repeat from any of the earlier steps with a new design alternative.

Important issues to note from this example are that multi-scale models have been used, data and knowledge from different disciplines have been used and, design/evaluation problem has been effectively used by solving a collection of sub-problems according to a pre-determined sequence. The final step (not shown) would be to select a few of the alternatives and perform the necessary experiments to validate the selection. Therefore, the experiments are done not to design the product but to verify the product. This approach has the potential to save time and money in bringing a chemical based product to the market. Obviously, the accuracy and range of application of the *v*PPD-lab software depends on the available data and models in the software.

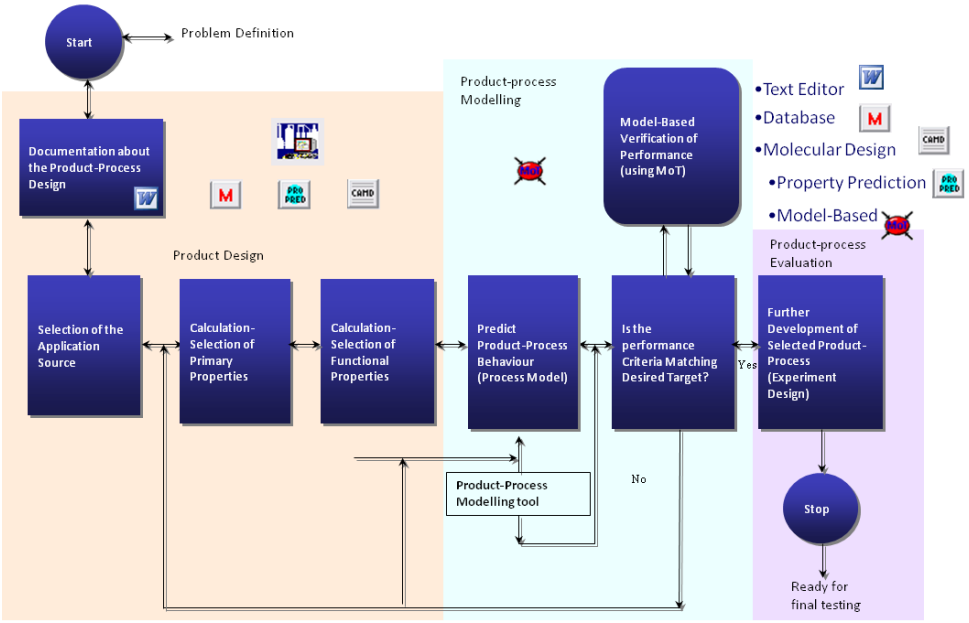



Figure 4.4c: The virtual product-process design lab

## 4.6 PC-SAFT Software Package (trial version)

This software performs multicomponent phase equilibrium calculations at given temperature with the PC-SAFT equation of state.

- The user firstly provides some information about the molecules involved in the mixture and gives the molar fraction of each of them. The temperature of the mixture is also required. Molecules may be chosen from an extended databank of nearly 1000 compounds (including some polymers) or may be created from $GC^{+}$ methods.
- Once the mixture completely described, the user chooses between two kinds of calculations:

**[1]** *bubble point calculation:* The mixture is assumed to be a saturated liquid. The software calculates the bubble pressure and the composition of the vapour phase in equilibrium (a single bubble in this case).

**[2]** *dew point calculation:* The mixture is assumed to be a saturated vapour. The software calculates the dew pressure and the composition of the liquid phase in equilibrium (a single droplet in this case).

### 4.7 SMSWIN

SMSWIN is a software package that Syngenta has given to CAPEC for maintenance, further development and integration with ICAS. SMSWIN has a database of compounds and their properties, a collection of property models for phase equilibrium calculations, which are especially suitable for solution properties involving solids. Currently, ProPred and the KT-UNIFAC model have been integrated with SMSWIN.

## 5. Research highlights (2008-2009)

The research highlights are discussed below in terms of new developments as well as publications record.

### 5.1 Summary of completed PhD research projects

#### *5.1.1 Computer aided design and analysis of reaction-separation and separation-separation systems - Piotr M. Mitkowski (PEC08-24)*

This work was concerned with the development and application of a general framework for design and analysis of integrated and hybrid chemical processes. Combination of at least two unit operations, based on different physical phenomena, is called a hybrid process since they jointly contribute to fulfill the process task. In principle, two types of hybrid processes were considered: reaction-separation where, for example, the combination of batch reaction and membrane-based separation was considered; and separation-separation where, for example, coupling of distillation with pervaporation was considered. An important issue in the design of hybrid chemical processes is the interdependency of the combined processes. Generally, design of hybrid chemical process involves an iterative, trial and error experiment-based procedure where the experience of process designer plays an important role. Since experiments are usually time consuming and expensive, the search space of the potential designs needs to be significantly limited. Therefore, applying a computer-aided and model-based framework can significantly help in searching the domain of potential process designs and significantly narrow down the search space, where further optimization and experimental efforts can be concentrated on.

The key factors for the design of hybrid chemical process are the identification of process boundaries, selection of feasible process combinations and the dependency of the performance between constituent processes. Therefore, using the developed framework consisting of three stages, (1) step-by-step methodology for design and analysis of hybrid chemical processes, (2) implementation, and (3) validation, it is possible to design the hybrid chemical process effectively.

The identification of process boundaries was performed in a conventional way, that is, by performing analysis of pure component properties and mixture analysis. The driving force approach was used to compare various separation techniques and to select the feasible combination of the processes. The derivative of the driving force with respect to composition of the key compound is used to identify the “bottleneck” of the separation technique. Therefore, a combination of this inefficient separation technique with another separation technique having a larger absolute driving force, will lead to a hybrid chemical process which is more efficient than any of the constituent separation techniques separately. For the purpose of simulation and evaluation of the designed hybrid chemical process, specific models were generated from a generic model, which represented the superstructure of two integrated processes. The application of the developed model-based framework was illustrated through five case studies involving reaction, distillation and membrane-based separation processes. In all case studies involving reaction, hybrid process configurations consisting of reactors and pervaporations integrated at different levels, were proposed. One of the hybrid chemical process designs has been verified experimentally. The framework is only limited by the availability of the property data of compounds, and models for separation and reaction models.

### *5.1.2 Identification for control - Jakob K Hussom (PEC08-26)*

This work was concerned with the optimization of the closed loop performance of controlled industrial processes. It was achieved through iterative schemes where input/output data were collected from the process during closed loop operation schemes for Iterative Feedback Tuning method was proposed.

In order to extend the application of this data driven tuning approach, the potential of Iterative Feedback Tuning was analyzed and tested for control structures where this tuning method was novel. Results have shown that the method is applicable for the nonlinear inventory control law and for a state space control system with state observes. For inventory control the proposal of applying a novel tuning method for the free parameters in the control law was interesting since classical tuning rules do not generally apply. The potential of the method was successfully illustrated by tuning step responses on a multivariable implementation of level control for a pilot scale four tank system. For the state space system analytical solutions to the feedback and the observer gain exist based on a plant model estimate. Tuning may therefore be relevant in case a mismatch exists between the true system and the model estimate used in the control design. The application of data driven tuning is interesting since most data driven approaches are focused on systems described by transfer functions. It was found that the Iterative Feedback Tuning can be applied for tuning, and that the gains converge to the known analytical solutions.

A general disadvantage in using the Iterative Feedback Tuning method is that a large number of plant experiments may be required, hence the rate of convergence is an important issue. Slow convergence rate is often seen when tuning for disturbance rejection due to insufficient excitation of the system. An algorithm (Perturbed Iterative Feedback Tuning), which balances the curvature of the cost function, rendering it less sensitive to noise, without introducing too much bias with respect to the optimum of the unperturbed problem, has been developed. Through this algorithm, it is possible to improve the rate of convergence by utilizing external perturbation signals during the data acquisition. Note that the external perturbations will affect the operating condition and hence the performance cost function. It was further shown that for minimum variance control an optimal perturbation signal design exists which does not bias the optimization.

### *5.1.3 Dynamic microfiltration: Critical flux and macromolecular transmission – Søren P Beier (PEC08-35)*

A dynamic microfiltration system, the *vibrating hollow fiber membrane module*, was investigated in this work. The system is thought to be coupled to the treatment of biological media, e.g. fermentation broth, from which macromolecules eventually continually should be removed. The advantages of dynamic membrane systems are the possibility of i) minimizing fouling problems, ii) probably lowering operational costs, and iii) enhancing macromolecular transmission.
A general introduction to pressure driven membrane processes was developed, followed by a review of different dynamic membrane filtration systems, reported in the scientific literature, with similarities to the experimental setup used in this project. Various aspects related to the dynamic microfiltration set-up used in the project were investigated: Critical flux measurement, determination of average surface shear rate, macromolecular transmission, and operation for extended periods. A method to measure macromolecular

adsorption on membranes was investigated. From the adsorption experiments, it was observed that irreversible adsorption strongly influences the hydraulic resistance of the membrane during operation. Furthermore, it was observed that sustainable operation is achievable since a sub-critical flux level is identifiable. One just has to define a "sustainable time period" in which process sustainability is to be evaluated. It was observed that sub-critical flux facilitates high and stable macromolecular transmission, and low and stable trans-membrane pressure (TMP). The critical flux is dependent on the degree of module vibrations, but whether the dependency of average surface shear rate is best described by shear-induced diffusivity or a power law correlation was found difficult of judge

### *5.1.4: Computer aided multiscale modeling for chemical product-process design – Ricardo Morales Rodriguez (PEC09-16)*

In the past, research in chemical engineering was more focused on the design, operation and optimization of the process, such as, petrochemicals and derivates (refineries, polymer plants, etc.). The main research goal usually was the efficient production of specific low-value but high-volume commodity chemicals. Product quality in this case was defined usually by its purity rather than its molecular structure. In the recent years, however, there has been an increased interest in product centric process design, operation, monitoring and control. There has also been a shift from process design, from low-value commodity chemicals to high-value structured/special chemicals and, from continuous to batch to hybrid processes. A noticeable feature of chemical product-centric process design is that the end-use (macro-scale) properties of the product-process define the design/control of the process, while the structure properties (micro-scale) define the design and performance of the product. For this reason a multiscale approach (from the modelling or experimental design point of view) has an important role in the management of the desired end-use characteristics of the product to be developed.

From a model based design (*virtual*) of the product, the use of multiscale models is essential in the preliminary design of the product, giving to the designer the capability to perform *virtual experiments* for the established work-flow (design steps). The use of mathematical models in general, and multiscale models in particular, imply the handling of complex models represented by sets of highly nonlinear partial- and ordinary- differential equations, and, algebraic equations. In virtual product design, properties at various scales need to be handled together with the mass, energy and/or momentum balance equations of different scales. That is, managing the complexity of the resulting models is an important issue.

The main contribution of this project is the introduction of a generic multiscale modelling framework for chemical product-process design, where a systematic workflow and data-flow is implemented to represent the different design steps. The multiscale modelling framework consists of four main steps: problem definition, product design, product-process modelling and, product-process evaluation; these steps involve the use of different computer-aided tools, such as, property prediction packages, molecular and mixture design tools, databases of chemical compounds, modelling tools, model-based libraries, tailor-made computer tools for specific models, commercial simulators (through CAPE-OPEN standards) and many more. As the computer-aided methods and tools come from different sources, they need to be properly integrated before being available in specific work-flow/data-flow schemes. The developed software, *Virtual Product-Process Design Lab* (*V*PPD-*l*) incorporates all of these and allows the designer to concentrate on making the

design decision. Through *V*PPD-*l*, a wide range of product-process design problems can be solved in a systematic and efficient manner. The use of the *Virtual Product Process-Design Lab* was illustrated through the design of three different products (case studies), all needing the use of the multiscale modelling features. The case studies are: direct methanol fuel cell, uptake of pesticides from water droplets on plants and controlled release of an active ingredient from polymeric microcapsules. These three case studies help to illustrate the use and reliability of the software and its application in the design of products with end-use characteristics. The introduction of the *Virtual Product-Process Design* opens a window of opportunities to be properly used in product development, design and education.

### *5.1.5: Development of group contribution$^{plus}$ models for prediction of properties of organic chemical systems – Hugo Edson Gonzalez Villalba (PEC09-17)*

Properties of chemicals are fundamental for the design and analysis of chemical, pharmaceutical, food, agrochemical and related industries. In order to meet the increased demand with respect to complexity of the chemical molecular structures, wider range of chemicals and accuracy, further development of existing property estimation methods and techniques and/or development of new models are necessary. The objective of this project was to develop new features for the existing property prediction methods.

The extended estimation methods need to be computationally simple and efficient, so they can be used routinely for process-product engineering calculations. Due to the fact that most of the molecular simulation approaches are far from being applied for thermodynamic modeling in conventional process simulators; thermodynamic models need to be fast and reliable to be used, and at the same time scale as the usual process calculations. Therefore, the group contribution approach, which has been finding increased use in both pure component and mixture property calculations, is considered as the basic model to improve. The main challenge here is to increase the applicability, accuracy and versatility of the group contribution (GC) models without requiring additional experimental data. The aim is the development of a hybrid model that combines molecular descriptors theory and group contribution methods for pure component and for mixture properties prediction. Models of this type are commonly known as GCPlus approach.

The main idea of this methodology is the use of connectivity indices (CI) to describe the molecular fragmentation that is characteristic for the UNIFAC group contribution method and that relates properties (molecular and atomic interactions in this case) with molecular structure. The result is the automatic generation of group interaction parameters (GIPs) for the UNIFAC group contribution method.

The original UNIFAC-CI (VLE and LLE) methods, together with the modified UNIFAC-CI (Dortmund) models were derived and the group definitions were defined in terms of stoichiometry and connectivity indices. Several examples highlighting the relation between group and connectivity indices parameters were shown, and the step-by-step calculation of the group interaction parameters was developed and illustrated. The application range was investigated and a set of basic rules and recommendations were proposed for the user.
The atom interaction parameter tables were developed through parameter estimation involving a database of measured binary VLE data for around 400 systems (covering UNIFAC groups, both functional and molecular). The correlation results were reasonably good in most cases. Also, the connectivity index-based UNIFAC group interaction parameters are tested for binary data sets not used for parameter optimization with good

results inside the application range. Some difficulties and inconsistencies were also investigated. These issues, such as why some systems did not report good results, when the extrapolations did not work, etc., are being investigated in a new PhD-project. This project is also extending the UNIFAC-Dortmund parameter tables for atom-interactions.

### 5.2 Publications record

The last 12-months have seen a big increase for CAPEC in the number of peer-reviewed journal publications (31 published since 2008 and 14 are in press/submitted) in the major chemical engineering journals (see Appendix 7.3), the number of plenary and keynote presentations (12) in international conferences and the total number of conference presentations (86 since 2008) in important international conferences. This has given CAPEC a greater visibility and attracted more attention to the research results published by CAPEC. CAPEC continues to have an open policy with respect to the publication of model parameters (especially, the CAPEC developed property models). The new version of ICAS 12.0, has all the latest property models and updated property model parameters.

## 6. Future Developments & Opportunities

Process systems engineering promotes the solution of a problem in a systematic manner. In this way, although it has traditionally been applied by the chemical engineering community to solve problems for the oil and petrochemical industries, its potential application range is much wider. This is because the word "process" also implies, among others, the process of solving a problem; design of a biochemical / biological process for conversion of biomaterial to specific chemicals; and, the process of finding/designing chemicals with desired properties.

Most of the earlier developments can be linked to chemical processes involved with the manufacture of high volume bulk chemicals and the related industries (such as the oil and gas, petrochemical and chemical industries). To a lesser extent, these methods and tools have also been applied to the manufacture of low volume specialty chemicals. Since its formation, CAPEC has contributed by providing systematic, reliable and efficient models, methods and tools that have now become standard for the chemical process industries as well as in chemical engineering education. CAPEC software, employing CAPEC models and methods, such as ProPred (property prediction software), ProCAMD (molecular design-solvent selection software), SustainPro (sustainable process design software), ProCAFD (process flowsheet design/synthesis), ICAS (Integrated Computer Aided System), are routinely used by the CAPEC consortium members and nearly 50 universities outside of Denmark.

The question therefore arises, what next? Where are the new challenges for CAPEC and what could be the new directions for research and education? Through collaboration with the CAPEC industrial member companies and academic partners, CAPEC conducted a "gap-analysis" with respect to identifying the current trends and the future needs with respect to chemical products, the processes that manufacture them and the models, methods and tools needed to design, analyze and operate them. The conclusions are briefly summarized below.

"*To satisfy the needs of the modern society, it is necessary to continuously develop better and significantly improved chemicals based products. The bulk chemicals as well as the specialty chemicals have important roles. For example, the bulk chemicals act as raw materials, solvents, process fluids, etc., are needed in the manufacture of specialty chemicals that may become an active ingredient for a pharmaceutical and/or drug product. Therefore improved designs of continuous processes (needed for the manufacture of bulk chemicals) are as important as designs of batch operations (needed for the manufacture of specialty chemicals).*"

Based on the above, CAPEC's future research will address the following questions:

- How does one identify the chemicals and their synthesis routes that will help to meet these demands, taking into account, also the questions of sustainability and protection of the environment (*eg.*, energy conservation and water resources)?
- How does one find their replacements and the processes to manufacture them? The sources for many of the raw materials used, especially those derived from oil, gas, and some plants/animals continue to be depleted and may soon be economically infeasible to use (*eg*., bio-refinery and green chemistry).

- How to develop and provide the necessary models, methods and tools through which the future problems can be addressed (*eg.*, multiscale modelling & integration/intensification)?

Thus, CAPEC plans to invest heavily in the following areas:
- Development of a generic computer aided modelling framework through which models of different forms and scale can be generated/created with significantly less time and resources than current practice.
- Use of a multidisciplinary approach because the process-product knowledge (including data) will come from different sources and the performance criteria, factors, etc., will involve other research groups (expertise). The opportunity for the CAPEC is that it can play the role of the "integrator" or "glue".
- Develop systematic solution approaches that combine methods and tools from different sources into problem specific flexible, reliable and efficient systems.

More specifically, for CAPEC to meet the challenges for the future, the following topics will have higher priority:
- computer aided frameworks for generation and use of multi-scale models (further extension of the predictive-generic property-product –process models)
- methods for design of experiments to collect and analyze data (efficient use of resources in data collection)
- methods & tools for process-product monitoring/control systems (and their design)
- sustainable process-product development (such as, hybrid processes, green chemistry, process intensification)
- systematic methods for product discovery (further extension of computer aided molecular and mixture design)

### 6.1 Managing the complexity through a systems approach

Product-process design and development in the life sciences, pharmaceutical, food and related industries, as opposed to the oil and petrochemical industries, is principally dependent on experiment-based trial and error approaches. Furthermore, unlike the oil and petrochemical industries in the life sciences, pharmaceutical, food and related industries, problems associated with product-process design and development involve, among others, the following distinct features:

- Multi-scale: important data related to the chemicals come from different sources, at different scales of time and size; for example, the properties that define the product characteristics are based on the microstructure of the molecule or material, while the process behaviour that needs to be monitored and controlled during operation is defined by the macroscopic (end-use) properties of the chemical system.
- Multidiscipline: the conversion of the biomaterial through biocatalysis requires knowledge of organic synthesis, enzymes, reaction catalysis, bioreactor design and operation – information about these topics come from different disciplines.
- Computer-aided techniques: lack of models to predict the behaviour of the chemicals at different scales, of enzymes during organic synthesis, of reaction kinetics, etc., means that appropriate model-based computer aided techniques have not been developed and use of experiment-based techniques is the only option.

Advances have been made on each of the above issues on specific areas of chemical and biochemical engineering. For example, multiscale polymerization reactors have been developed to investigate the operation of reactors; techno-economic assessment related to sustainability biofuels have been made using data from engineers, economists and scientists; computer-aided systems have been developed to perform routine mass and energy balances of chemical and biochemical processes. The demand for improved chemical-based products, made from more sustainable raw material resources and employing more efficient processes to make them, however, requires the above issues and others to be tackled in an integrated manner. This means that methods and tools suitable for current and future product-process development need to manage complex situations that require handling of data and knowledge from different sources and at different time and size scales. That is, the dimensions of the problems we need to solve have become larger. Therefore, a systems approach that can efficiently "manage the complexity" becomes very desirable.

The multi-dimensional and multi-scalar nature of problems is highlighted through Fig. 5, where, it can be noted that at the micro- and meso- scales, the related problems are dealing with the microstructure of the molecules or materials and their properties; at the macro-scale (traditional area of application of chemical engineering), the related problems are mainly dealing with the process and its operation to produce a desired chemical; at the mega-scale, the related problems are, among others, dealing with enterprise wide optimization and supply chain issues. Many of the problems of current interest, such as, finding the optimal biorefinery, sustainable chemical process-product design, use of green solvents, process (energy and water) integration, etc., involve the macro- and mega-scales.

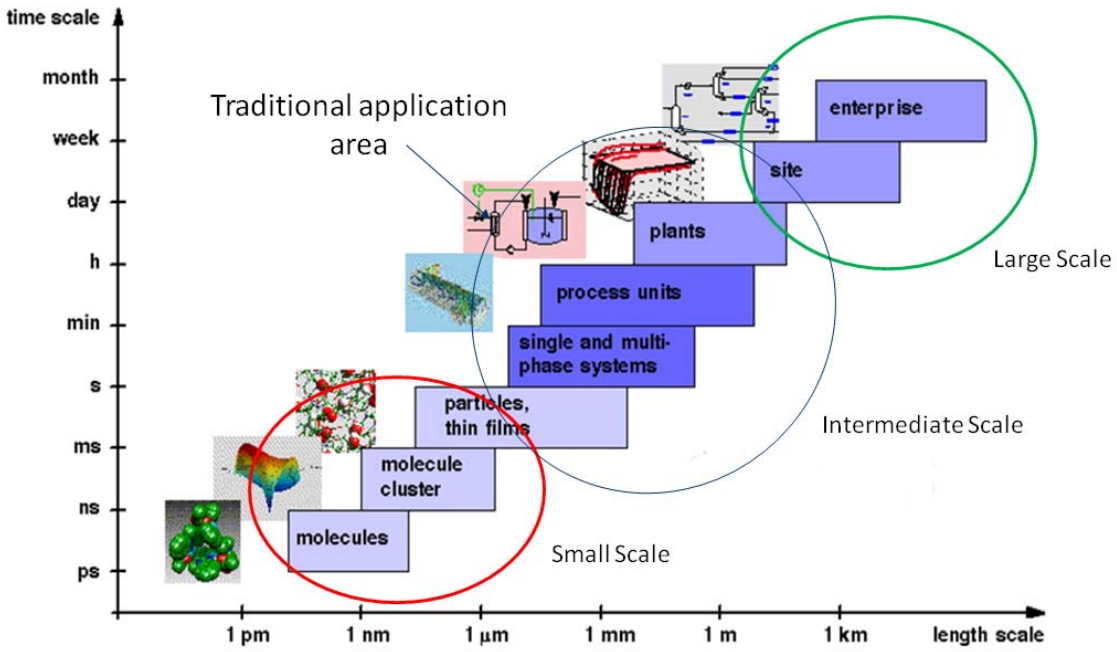



Figure 5: Multiscale nature of product-process design problems

To manage the complexity, a systems approach would develop a framework (the architecture of the software) for handling the diverse set of methods and tools needed to

solve a wide range of problems, for a potential computer-aided system. Such systems need to have a knowledge base of data (for example, of the active ingredients, solvents, polymers, etc.); a library of models (for example, models to predict properties – in case data is not available - of active ingredients, solvents, polymers, etc.; models to predict the controlled release from the microcapsule; models to predict the behaviour of the mixing process); a design method (for example, guiding the engineer/scientist through the sequence of steps needed to identify the best solution); and, other associated methods-tools (such as a tool to analyze data; a tool to create the missing model; a tool to screen feasible alternatives). The principal idea here is to decompose a complex problem into a set of sub-problems that are easier to solve and identify those that can be solved through model-based solution approaches. Solving these sub-problems according to a pre-determined sequence helps to reduce the search space through each subsequent sub-problem solution, until a sub-problem cannot be solved with models anymore. At this point, the experiment-based trial and error approach takes over to determine the final solution. The advantage of this combined hybrid (systems approach) is that during the early stages, where enough data and models are available (or could be easily generated), the search space is rapidly reduced. In the later stages, where quantitative values become important and data/models become more unreliable, the experimental resources are employed, sometimes only to evaluate a few feasible alternatives to identify the truly innovative and best solution. Several examples of such computer aided systems can be found at CAPEC and current research is expanding on this approach through the development of a collection of methods and tools.

### 6.2 Some specific plans (CAPEC coworkers) for the future

Within the next 6-months, CAPEC will start 3-4 PhD projects in the areas of energy; product-process design; multiscale modelling; modelling, design, control under uncertainty; and solvent based organic synthesis. Also, 2 post-doctoral projects will be started in the area of modelling (Dr. Ricardo Morales-Rodriguez) and, PAT and process monitoring (Ravendra Singh). At least one MSc-level project on computer-aided product design will be started.

## 7. Appendix

### 7.1 Membrane lab

*List of experiments:*

| Experiment Type | Experiment objective (measure) |
|---|---|
| Pressure driven | Water permeability |
| | Solute permeability |
| | Membrane selectivity/retention |
| | Gas permeability |
| Concentration driven | Osmotic water permeability |
| | Solute permeability |
| | Time-lag measurements and/or sorption-desorption measurements (diffusion coefficients, distribution coefficients) |
| Partial pressure driven | Water (vapor) permeability |
| | Solute (vapor) permeability |
| | Concentration factor/separation factor |
| Electrical potential driven | Electrical permeability/resistence |
| | Solute permeability |
| | Electro-osmotic water permeability |

*List of equipments:*

| Type of equipment | Remarks |
|---|---|
| Various flat sheet flow cell plants | Pressurized cells for nano-filtration (NF), ultra-filtration (UF), micro-filtration (MF), reverse-osmosis (RO) |
| | Diffusion and reverse osmosis cells |
| Ultra-filtration/micro-filtration hollow fiber module plants | High frequency back-pulsing operation |
| | High frequency vibration operation |
| Electro-ultrfiltration test plant | |
| Lab-20 pilot module | For RO, NF, UF, MF |
| M38/M39/4" – spiral wound module | DSS |
| Membrane distillation test plants | Pervaporation, vacuum membrane distillation |
| | Direct contact membrane distillation, sweeping gas membrane distillation, osmotic membrane distillation |
| Test cells | Electrodialysis |
| Pilot plant | Electrodialysis |
| Casting equipment | Membranes |
| Modification equipment/machine | UV |
| Analytical instruments | *HPLC/SEC with RI and UV detectors* |
| | Conductivity meters |
| | Polarimeter |
| | UV instrument |

## 7.2 CAPEC Control Lab

The main purpose of the CAPEC Control Lab is to give our students hands-on experience with process control problems. The laboratory is presently undergoing a complete renovation.

Two facilities are in use:

- a 4-tank exercise, and
- a distillation column

With the 4-tank exercise (used as a 2-tank system), students make two experiments. The first day they determine the dynamics of the system. Then they go to the computer lab to configure a PI-controller by simulation. On the second day they try out their controller settings on the real system. This setup is used in all our introductory teaching; about 75 students each year.

A HTST pasteurizer has also been established

The distillation column is used in an intensive 3-weeks course. This course teaches the participants to:

- Plan and execute start-up of the chemical plant.
- Apply a Distributed Control System for chemical plant operation.
- Simulate and document the operation of a chemical plant.
- Reason on process behaviour during start-up and operation.

4 tank exercise

HTST pasteurizer

Indirect Vapour Recompression Distillation Pilot Plant

### 7.3 CAPEC publication list (2008-2009)

| | **A - Ph.D. Theses and Monographs** |
|---|---|
| PEC08-01 | Vipasha Soni, 2008, ”Chemically Structured Products: Simultaneous model-based design of process and assisting structured materials”, Ph.D. thesis |
| PEC08-23 | Florin Paul Davidescu, 2008, “Optimal Experimental Design for Grey-Box Models”, Ph.D. thesis |
| PEC08-24 | Piotr Tomasz Mitkowski, 2008, “Computer aided design and analysis of reaction-separation and separation-separation systems”, Ph.D. thesis |
| PEC08-26 | Jakob Kjøbsted Huusom, 2008, “Identification for Control”, Ph.D. thesis |
| PEC08-35 | Søren Prip Beier, 2008, “Dynamic Microfiltration: Critical flux and macromolecular transmission”, Ph.D. Thesis |
| PEC09-01 | Maria Antonieta Alvarez Villanueva, Stuart M. Stocks and Sten Bay Jørgensen, **2009**, ”Bioprocess Modelling for Learning Model Predictive Control (L-MPC)”, in: “Computational Intelligence Techniques for Bioprocess Modelling, Supervision and Control”, M.C.Nicoletti and L.C. Jain (Eds.), Studies in Computational Intelligence, Springer-Verlag, Germany, Chapter 9, pp. 237-280 |
| PEC09-16 | Ricardo Morales Rodriquez, **2009**, “Computer-Aided Multiscale Modelling for Chemical Product-Process Design”, Ph.D. thesis |
| PEC09-17 | Hugo Edson Gonzalez Villalba, **2009**, “Development of Group Contribution$^{plus}$ Models for Properties of Organic Chemical Systems”. Ph.D. thesis |

| | **B - Reviewed publications in International Journals** |
|---|---|
| PEC06-40 | Bao Lin, Claude F. Leibovici, Sten Bay Jørgensen, 2008, "Optimal Component Lumping: problem formulation and solution techniques", Computers and Chemical Engineering, Vol. 32, number 6, pp. 1167-1172 |
| PEC07-09 | Odgaard, P. F. and Lin, B. and Joergensen, S.B., 2008, "Observer and data-driven model based fault detection in Power Plant Coal Mills", IEEE Transactions on Energy Conversion, 23(2), pp. 659-668 |
| PEC07-10 | Florin Paul Davidescu and Sten Bay Jørgensen, 2008, "Structural parameter identifiability analysis for dynamic reaction networks", Chemical Engineering Science, 63, pp. 4754-4762 |
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| F | Mohammad Shafique Bashir and Rafiqul Gani, 2008, "A Systematic Methodology for the Selection of Green and Non-Reactive Solvents for Multistage Organic Reactions", CAPE-Forum, Thessaloniki, Greece, 6-9 February |
| F | Naweed Al-Haque and Rafiqul Gani, 2008, "Biorefinery: Analysis of Process Design Alternatives", CAPE-Forum, Thessaloniki, Greece, 6-9 February |
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| F | R. Gani, Ravendra Singh, Krist V. Gernaey, 2008, "A model-based framework for design and analysis of PAT systems", 1st European Conference on Process Analytics and Control Technology, EuroPact 2008, Frankfurt am Main, Germany, 22-25 April **(Plenary Lecture)** |

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| F (Poster) | Merlin Alvarado-Morales, Naweed Al-Haque, Krist V. Gernaey, John M. Woodley, Rafiqul Gani, 2008, “CAPE Methods and Tools for Systematic Analysis of New Chemical Product Design and Development”, ESCAPE-18, Lyon, France, 1-4 June |
| F | Ravendra Singh, Krist V. Gernaey, Rafiqul Gani, 2008, “Off-line design of PAT systems for on-line applications”, ESCAPE-18, Lyon, France, 1-4 June |
| F | Ana Carvalho, Rafiqul Gani , Henrique A. Matos, 2008, “Systematic methodology for process analysis and generation of sustainable alternatives”, ESCAPE-18, Lyon, France, 1-4 June |
| F (Poster) | Kavitha Chelakara Satyanarayana, Jens Abildskov, Rafiqul Gani, 2008, “Computer Aided Polymer Design using Group Contribution plus Property Models”, ESCAPE-18, Lyon, France, 1-4 June |
| F | Rafiqul Gani, 2008, “A Model-Based Systems Approach for Integrated Chemical Product-Process Design”, Process Development Symposium 2008, Jiminy Peak Resort, The Berkshires, Hancock, MA, USA, 22-25 June **(Plenary Lecture)** |
| F | Oscar Barrero Mendoza and Sten Bay Jørgensen, 2007, ”Multirate Process Data Assimilation using the Extended Kalman Filtering”, IFAC World Congress, Seoul, 6-11 July |

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| F | Gunnar Jonsson, 2008, "Modelling aroma stripping under various forms of membrane distillation processes", International Conference on membranes and membrane processes: ICOM2008, Hawaii, USA, 12-18 July **(Keynote lecture)** |
| F | Gunnar Jonsson, 2008, "Tuning of the cut-off curves by dynamic microfiltration", International Conference on membranes and membrane processes: ICOM2008, Hawaii, USA, 12-18 July |
| F | Søren Prip Beier, Gunnar Jonsson, 2008, "Dynamic microfiltration: Investigation of critical flux measurement methods and improved macromolecular transmission", International Conference on membranes and membrane processes: ICOM2008, Hawaii, USA, 12-18 July **(Keynote lecture)** |
| F | Mohd. Kamaruddin Abd. Hamid, Rafiqul Gani, 2008, "A model-based methodology for simultaneous process design and control for chemical processes", FOCAPO 2008 (Foundations of Computer-Aided Process Operations), Cambridge, Boston, Massachusetts, USA, June 29 - July 2, 2008 |
| F | Ana Carvalho, Henrique Aníbal Matos, Rafiqul Gani, 2008, "Systematic Methodology for Continuous/ batch processes: analysis and generation of sustainable alternatives", FOCAPO 2008 (Foundations of Computer-Aided Process Operations), Cambridge, Boston, Massachusetts, USA, 29 June – 2 July 2008 |
| F | Rafiqul Gani, 2008, "The Need and Use of Thermophysical Databases in Property Modeling and for Applications in Process-Product Design", CALCON 2008, The 63rd Colorimetry Conference, Hyatt Regency Jersey City on the Hudson, Jersey City, New Jersey, USA, 2-6 July **(Plenary Lecture)** |
| F<br>(Poster) | Oscar Andres Prado Rubio, Sten Bay Jørgensen and Gunnar Jonsson, 2008, "Integrated Bioreactor and Membrane Separation Processes", ISGSB-08, Helsingør, Denmark, 17-20 August |
| F | Gunnar Jonsson, 2008, "Dynamics of the ultrafiltration process", 11th Nordic Filtration Symposium, IDA, Copenhagen, Denmark, 25-26 August, **(Keynote lecture)** |
| F | R. Fuhlendorff, J.-U. Rype, A. Garde, A. Vrang, S. Madsen, G. Jonsson, 2008, "Combining Membrane Separation and Fermentation Processes for improved performance", 11th Nordic Filtration Symposium, IDA, Copenhagen, Denmark, 25-26 August |
| F | Søren Prip Beier, Gunnar Jonsson, 2008, "A vibrating membrane bioreactor (VMBR): Macromolecular transmission – influence of extracellular polymeric substances", 11th Nordic Filtration Symposium, IDA, Copenhagen, Denmark, 25-26 August |
| F | R. Gani, 2008, "A process systems engineering approach for managing the complexity", ChemPor 2008, 10th International Chemical and Biological Engineering Conference, Braga, Portugal, 4-6 September **(Plenary Lecture)** |
| F | Hugo E. González, Jens Abildskov, Rafiqul Gani, 2008, "Computer-aided Phase Equilibria Prediction for Organic Systems: UNIFAC-CI. Analysis, Revision and Extention", ChemPor 2008, 10th International Chemical and Biological Engineering Conference, Braga, Portugal, 4-6 September |
| F | Ricardo Morales-Rodríguez, Rafiqul Gani, 2008, "Systematic Modelling Framework in Chemical Product-Process Design and development", ChemPor 2008, 10th International Chemical and Biological Engineering Conference, Braga, Portugal, 4-6 September |
| F | Netta Liin Rossing, Morten Lind, Niels Jensen and Sten Bay Jørgensen, 2008, "A Goal Based Methodology for HAZOP Analysis", CSEPC conference, Harbin, China, 8-10 September |

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| F | Tolga Us, Niels Jensen, Morten Lind, Sten B. Jørgensen, 2008, "Fundamental Principles of Alarm Design", CSEPC conference, Harbin, China, 8-10 September |
| F | Oscar Andres Prado Rubio, Sten Bay Jørgensen, Gunnar Jonsson, 2008, "Modelling of Electrically Driven Membrane Separation Processes", BEC08, Supetar, Croatia, 17 September |
| | Gernaey K.V., Sin G., Albo E., Woodely J.M., Singh R., Gani R., 2008, "Application of mechanistic models within a PAT framework", ISPE conference, Malmø, Sweden, 1 October |
| F | R. Gani, J.M. Woodley, 2008, "Development of sustainable chemical processes", RES & QUIMICA-08, III Int. Symp. of Chemical Industry and Waste, Barcelona, Spain, 22-23 October **(Invited Lecture)** |
| F | Rafiqul Gani, Concepcion Jimenez-Gonzalez, David Constable, Muhammad Shafique Bashir, 2008, "Solvents In Organic Synthesis: Replacement and Multi-Step Reaction Systems", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Kavitha Chelakara Satyanarayana, Jens Abildskov, Rafiqul Gani, Georgia Tsolou, Vlasis Mavrantzas, 2008, "Atomistic Simulation of the Diffusion of Small Gas Molecules in Polyisobutylene", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Hugo E. González, Jens Abildskov, Rafiqul Gani, Tariq A. Khan, Sabyasachi Sen, David Bluck, 2008, "Increased Application Range of Property Models without New Experimental Data", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Rafiqul Gani, 2008, "Property Model Analysis for Use In Process-Product Development", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Oscar A. Prado, Sten B. Jørgensen, Gunnar Jonsson, 2008, "Modelling of Ion Transport across Anion Exchange Membranes Under Current Reversal Conditions", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Ricardo Morales-Rodríguez, Rafiqul Gani, 2008, "A Systematic Multiscale Modelling Framework for Product-Process Design and Development", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Sten Bay Jorgensen, 2008, "Reactor Modelling for Monitoring and/or Multivariable Control - a Process Analytical Tool", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Iskandar Halim, Ana Carvalho, Rajagopalan Srinivasan, Rafiqul Gani, Henrique A. S. Matos, 2008, "Sustainability Analysis of Chemical Process Plants Using a Hybrid Heuristic and Indicator Model", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Mengzhe Wu, John Bagterp Jørgensen, Sten Bay Jørgensen, 2008, "A Dynamic Model for a Cupola Furnace", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Elisa Conte, Ricardo Morales-Rodriguez, Rafiqul Gani, 2008, "The Virtual Product-Process Design Laboratory", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Kavitha Chelakara Satyanarayana, Jens Abildskov, Rafiqul Gani, Georgia Tsolou, Vlasis Mavrantzas, 2008, "Computer Aided Polymer Design Using Multiscale Modeling", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Ravendra Singh, Krist V. Gernaey, Rafiqul Gani, 2008, "A Model-Based Framework for Systematic Product Quality Monitoring and Control", AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |

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| F | Merlín Alvarado-Morales, João Terra, Krist V. Gernaey, John Woodley, Rafiqul Gani, 2008, ”Bioprocess Synthesis, Design and Analysis through a Group-Contribution Approach”, AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| Poster | Ana Carvalho, Henrique A. S. Matos, Rafiqul Gani, 2008, “Design of Sustainable Chemical Process: Systematic Retrofit Analysis Generation and Evaluation of Alternatives”, AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| Poster | Martin E. Christensen, Jens Abildskov, John P. O'Connell, 2008, “Recent Developments in Excess Solubility Estimations - Solute-Free Nonideality”, AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| Poster | Pertti S. Koukkari, Risto Pajarre, Rafiqul Gani, 2008, “Use of the Constrained FREE Energy Method for Multiphase Chemical REACTOR Simulation”, AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| Poster | Ravendra Singh, Krist V. Gernaey, Rafiqul Gani, 2008, “A Software Tool for Design of Process Monitoring and Analysis Systems”, AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Maria Antonieta Alvarez Villanueva, Stuart M. Stock, Sten Bay Jørgensen, 2008, ”Reactor Modelling for Monitoring and/or Multivariable Control – A Process Analytical Tool”, AIChE Annual Meeting 2008, Philadelphia, PA, USA, 16-21 November |
| F | Jakob Kjøbsted Huusom, Håkan Hjalmarsson, Niels Kjølstad Poulsen and Sten Bay Jørgensen, 2008, “Improving Convergence of Iterative Feedback Tuning using Optimal External Perturbations”, 47th IEEE Conference on Decision and Control, Cancun, Mexico, 9-11 December |
| F | Rafiqul Gani, 2008, “Models, modelling and Chemical Engineering – What Next?”, ICChE (International Congress of Chemical Engineering) 2008, Dhaka, Bangladesh, 31 December 2008 – 1 January 2009 **(Plenary Lecture)** |
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| | **F - Conference Presentations 2009** |
| F | Jamal Rashed and Rafiqul Gani, 2009, “Model-based retrofit design and analysis of petrochemical processes”, in Proceedings of 1st Annual Gas Processing Symposium, Doha, Qatar, 10-12 January |
| F | Sten Bay Jørgensen, 2009, “Modelling for Process and Control Design”, Nordic Process Control Workshop ’09, NPCW09, Porsgrunn, Norway, 29-30 January |
| F | Oscar Andres Prado Rubio, Sten Bay Jørgensen, Gunnar Jonsson, 2009, “Modeling Reverse Electro-Enhanced Dialysis for Integration with Lactic Acid Fermentation”, Nordic Process Control Workshop ’09, NPCW09, Porsgrunn, Norway, 29-30 January |
| F | Jakob Kjøbsted Huusom, Håkan Hjalmarsson, Niels Kjølstad Poulsen, Sten Bay Jørgensen, 2009, “Pertubed Iterative Feedback Tuning”, Nordic Process Control Workshop ’09, NPCW09, Porsgrunn, Norway, 29-30 January |
| F | Sten Bay Jørgensen, 2009, “Modelling Paradigms for Process Design, Identification and Control”, MIC´09: Modelling, Identification and Control, IASTED conference, Innsbruck, Austria, 16-18 February **(Invited Keynote Lecture)** |
| F | R. Singh, K. V. Gernaey, R. Gani, 2009, “ICAS-PAT: A new software tool for systematic design/validation of process monitoring and analysis systems (PAT systems)”, APACT-09, Glasgow, UK, 5-7 May |
| | **AMIDIQ, Mazatlan, Mexico, 19-22 May – 4 presentations** |

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| F | Rafiqul Gani, 2009, "Managing the complexity in product-process design", AMIDIQ XXX (Academia Mexicana de Investigación y Docencia en Ingenería Química 2009), Mazatlan, Mexico, 19-22 May **(Plenary Lecture)** |
| F | Carlos A. Diaz-Tovar, Roberta Ceriani, Rafiqul Gani and Bent Sarup, 2009, "Simulation and Optimization of a Solvent Recovery Process in the Vegetable Oil Industry", AMIDIQ XXX (Academia Mexicana de Investigación y Docencia en Ingenería Química 2009), Mazatlan, Mexico, 19-22 May |
| F | Alicia Román Martínez, Rafiqul Gani, John M. Woodley, 2009, "Design methodology for intensified bioprocesses", AMIDIQ XXX (Academia Mexicana de Investigación y Docencia en Ingenería Química 2009), Mazatlan, Mexico, 19-22 May |
| F | Ricardo Morales-Rodríguez, Rafiqul Gani, 2009, "Product-Process Design Multiscale Modelling Framework", AMIDIQ XXX (Academia Mexicana de Investigación y Docencia en Ingenería Química 2009), Mazatlan, Mexico, 19-22 May |
| | **FOCAPD-2009, Colorado, USA, 7-12 June – 3 presentations** |
| F | Mohd Kamaruddin Abd Hamid, Gurkan Sin, Rafiqul Gani, 2009, "Determination of optimal design and control decisions for reactor-separator systems with recycle", Foundations of Computer-Aided Process Design (FOCAPD) 2009, Breckenridge, Colorado, June 7 – 12 |
| F | Gürkan Sin, Anne S Meyer, Krist V. Gernaey, 2009, "Are mechanistic cellulose-hydrolysis models reliable for use in biofuel process design? –identifiability and sensitivity analysis", Foundations of Computer-Aided Process Design (FOCAPD) 2009, Breckenridge, Colorado, June 7 – 12 |
| F | Ana Carvalho, Henrique A. Matos, Rafiqul Gani, 2009, "Analysis and generation of sustainable alternatives: Continous and batch processes using SustainPro", Foundations of Computer-Aided Process Design (FOCAPD) 2009, Breckenridge, Colorado, June 7 – 12 |
| | **ESCAPE-19, 2009, Cracow, Poland, 14-17 June – 10 presentations** |
| F | Ricardo Morales-Rodríguez, Rafiqul Gani, 2009, "Multiscale Modelling Framework for Chemical Product-Process Design", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 13-17 June |
| F | Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen, 2009, "Data Driven Tuning of State Space Control loops with unknown state information and model uncertainty", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 13-17 June |
| F | Elisa Conte, Ricardo Morales-Rodriguez, Rafiqul Gani, 2009, "The Virtual Product-Process Design Laboratory as a Tool for Product Development", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 13-17 June |
| F | Ravendra Singh, Krist V. Gernaey, Rafiqul Gani, 2009, "A software tool for design of process monitoring and analysis systems", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 13-17 June |
| F | Oscar Andres Prado-Rubio, Sten Bay Jørgensen, Gunnar Jonsson, 2009, "Lactic Acid Recovery in Electro-Enhanced Dialysis: Modelling and Validation", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 13-17 June |
| F | Mohd. Kamaruddin Abd Hamid, Gurkan Sin, Rafiqul Gani, 2009, "A new model-based methodology for simultaneous design and control of reaction-separation systems with recycle", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 13-17 June |

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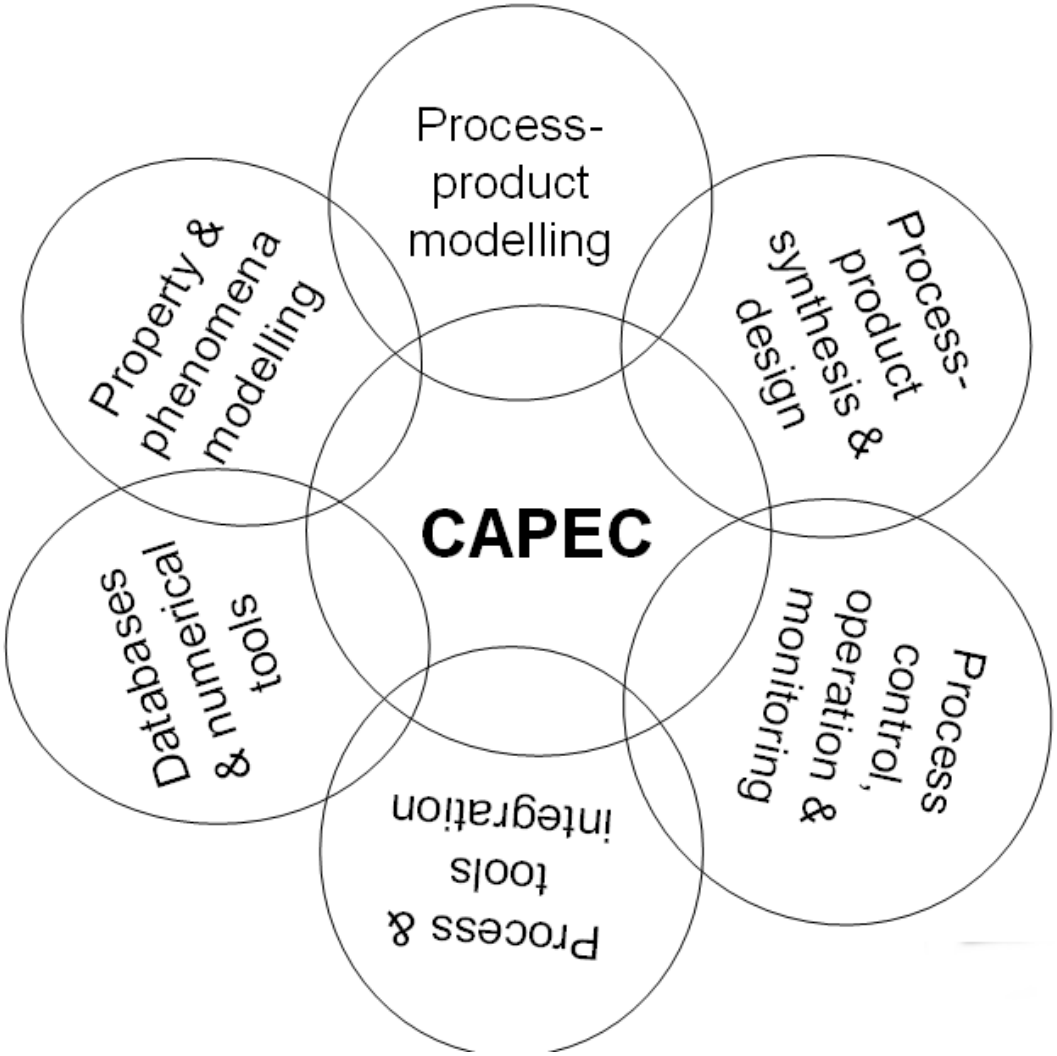
| F | Gürkan Sin, Krist V. Gernaey, 2009, "Improving the Morris method for sensitivity analysis by scaling the elementary effects", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 13-17 June |
| F | Netta Liin Rossing, Morten Lind, Niels Jensen and Sten Bay Jørgensen, 2009, "A Goal Based HAZOP Assistant", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 13-17 June |
| F | Jamal Rashed, Rafiqul Gani, 2009, "Model-based retrofit design and analysis of petrochemical processes", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 13-17 June |
| F | Pimporn Lek-utaiwan, Rafiqul Gani, Bunyaphat Puphnit, Nakarin Mongkolsiri, 2009, "Integrated design of solvent based extractive separation processes including experimental validation", 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 13-17 June |
| | **17th Symposium on Thermophysical Properties, Boulder, CO, USA, 21-26 June – 1 presentation** |
| F | Martin Ellegaard, Jens Abildskov, John O'Connell, 2009, "Solubility of solids in mixed solvents – modeling and data reduction", Seventeenth Symposium on Thermophysical Properties, Boulder, CO, USA, 21-26 June |
| F | Romain Privat, Rafiqul Gani and Jean-Noël Jaubert, 2009, "Prediction of thermodynamic properties of pure components and mixtures: cubic equations of state versus molecular theory-derived equations of state: a short comparison", JETC10, Copenhagen, 22-24 June |
| | **ESAT-2009, 27 June- 1 July – 3 presentations** |
| F | Martin Ellegaard, John O'Connell, Jens Abildskov, 2009, "Corresponding states correlation for liquids densities and gas solubilities in ionic liquids", 24th European Symposium on Applied Thermodynamics, ESAT-2009, Santiato de Compostela, Spain, 27 June – 1 July |
| F | Romain Privat, Rafiqul Gani and Jean-Noël Jaubert, 2009, "Application of the GC-plus approach to PC-SAFT EOS and prediction of phase Equilibria", 24th European Symposium on Applied Thermodynamics, ESAT-2009, Santiato de Compostela, Spain, 27 June – 1 July |
| F | Roberta Ceriani, Elisa Conte, Martin Dela Ellegaard, Carlos A. Diaz-Tovar, Cintia B. Gonçalves, Antonio J.A. Meirelles, Rafiqul Gani, 2009, "GC, $GC^+$ (Group Contribution Plus) and Atom Connectivity Index-Based Models for Physical Properties of Lipid Systems", 24th European Symposium on Applied Thermodynamics, ESAT 2009, Santiago de Compostela, Spain, 27 June-1 July |

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